Introduction to Quantum Optics

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Preface.

- Version history:
  (1) Version 0.1 (2024.06.09–2024.09.19): Chapter 1–12, Appendices.
  (2) Version 0.2 (2024.09.19–2024.09.26): Added Chapter 13 and many other updates.
    (a) Version 0.2.1 (2024.09.26–2024.10.02): Bug fixes.
    (b) Version 0.2.2 (2024.10.02–2025.01.26): Bug fixes, stressed difference between position vector $\boldsymbol{r}$ and "position" variable q, changed the names of q and p to q-quadrature and p-quadrature to avoid confusion.
  (3) Version 0.3 (2025.01.26–2025.04.15): Updated Sec. 3.3 to emphasize difference between Q-numbers and c-numbers, added Exercise 3.10 there. Extended Exercises 4.3 and 4.22. Added Exercise 4.20. Added Sec. 6.6.2 to explain the Schrödinger picture of a beam splitter. Updated Sec. 7.2 about the Schrödinger picture of loss. Updated Sec. 9.3 and added Exercise 9.2. Updated Sec. 10.3. Updated Eqs. (12.9)–(12.13). Rewritten Sec. 12.2 to frame Bell's theorem in terms of the CHSH game. Updated Exercise D.6 and added solution in Appendix K. Bug fixes.
    (a) Version 0.3.1 (2025.04.16–2025.04.28): Distinguished side notes and remarks (remarks clarify common issues and misconceptions). Format tweaks. Minor updates.
  (4) Version 0.4 (2025.04.28–2025.07.31): Added appendices on statistics and open quantum systems. Significant update of the appendix on probability. Updated Chap. 2 and 3 to stress that modes are degrees of freedom. Switched to `newtxtext` typeface for the text.
- **Advanced topics are denoted by ***; I no longer bold the vectors in them.
- Acknowledgments: TODO
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Contents

CHAPTER 1

Why Study Quantum Optics?

I'll tell you the elephant in the room upfront: No major industry, apart from the academia and a few startups (e.g., https://www.idquantique.com/, https://www.xanadu.ai/, https://www.psiquantum.com/), currently requires their employees to know quantum optics.

Classical optics, together with some rules of thumb, such as the quantization of electromagnetic energy and the existence of spontaneous emission, are enough to describe every major optical technology that exists today (e.g., cameras, light-emitting diodes, solar cells, photodetectors, lasers, optical communications, photolithography). In other words, if you won't be doing physics for research, it is enough to stick with Maxwell's equations and the early quantum theory invented by Planck ($E = nh\nu$) and Einstein (the phenomena of absorption, stimulated emission, and spontaneous emission) [1]. A lot of quantum effects, even the photoelectric effect [2], can be explained without quantizing the EM fields.

If you will be doing research, however, then studying quantum optics is a no-brainer, as it is a **gateway** to many fields of physics at the graduate level:

(1) Quantum optics is an important example of **quantum field theory**. According to the standard model, everything in physics (bar gravity) is a quantum field, and quantum optics, i.e., the quantum theory of electromagnetic fields, is the first example you will likely learn.

(2) Many important experiments in **quantum information** and **quantum foundations** rely on quantum optics. For example, you need quantum optics to describe how **quantum key distribution** works and experiments there are all based on quantum optics.

Quantum optics experiments have also been used to test some fundamental properties of physics, as recognized by the 2012 and 2022 Nobel prizes (https://www.nobelprize.org/prizes/physics/2012/summary/ and https://www.nobelprize.org/prizes/physics/2022/summary/).

A founder of quantum optics, Roy Glauber, has won a Nobel prize as well (https://www.nobelprize.org/prizes/physics/2005/summary/).

(3) **Quantum measurement theory** and **open quantum system theory** are often studied in conjunction with quantum optics because examples in those theories are most commonly demonstrated with quantum optics experiments—see, again, the 2012 Nobel prizes for example (https://www.nobelprize.org/prizes/physics/2012/summary/).

(4) **Gravitational-wave detectors** are giant Michelson optical interferometers that detect tiny movements in the mirrors due to gravitational waves, and they are now so sensitive that they are limited by the fundamental quantum fluctuations of the light beams. A quantum technique called optical squeezing is now being used to reduce the quantum fluctuations (https://www.ligo.org/science/Publication-SqueezedVacuum/).

In general, the study of sensors at the fundamental quantum level is called **quantum metrology**, and it is often studied in conjunction with quantum optics because optical sensors are arguably the most important application of quantum metrology (gravitational-wave detection, telescopes, microscopes, etc.). The probabilistic nature of quantum mechanics place fundamental limits to the sensor precision, and we need a quantum theory of light if we want to derive those fundamental limits and find out how the sensors can be improved in the presence of quantum effects.

(5) In **deep-space optical communication** (https://www.nasa.gov/mission/deep-space-optical-communications-dsoc/), the received optical signal on earth or satellite is so weak that one must

design the system and the measurement carefully in accordance with quantum optics to minimize quantum sources of noise [3].

(6) Most quantum experiments in research with atoms, ions, or superconducting circuits, e.g., for quantum computing, use optical beams or microwaves as **probes** to measure and control the systems, and a quantum theory of light is often needed to make the theory of **light-matter interaction** consistent.

Experiments on light-atom interactions have won a few Nobels as well (https://www.nobelprize.org/prizes/physics/1997/summary/, https://www.nobelprize.org/prizes/physics/2012/summary/).

(7) Besides atoms, ions, and superconducting circuits, people have also proposed the use of photonics (optical devices) for quantum computing (see, e.g., https://www.xanadu.ai/, https://www.psiquantum.com/).

Will any of these quantum technologies become a major force in the future industry? I don't know and I cannot promise anything. The economic factor should not be the main reason you study quantum optics anyway. Apart from research, here are some noble reasons why one may want to study quantum optics:

(1) You like optics and just want to learn more about it.
(2) You are deeply annoyed that classical electromagnetism is unable to predict the quantization of electromagnetic energy.
(3) You are deeply curious how electromagnetism can be generalized and combined with the quantum theory invented by Schrödinger and Heisenberg. You want your physics unified under one formalism and don't want just a bunch of seemingly arbitrary rules, like the early quantum theory by Planck and Einstein.
(4) You want a taste of quantum field theory, quantum measurement theory, and open quantum system theory.

In other words, curiosity should be your reason. If you have it, I welcome you to this course.

CHAPTER 2

Classical Electromagnetism (EM)

2.1. Classical EM and what's wrong with it

Classical electromagnetism (EM) is specified by four Maxwell's equations:

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0}, \qquad \nabla \cdot \boldsymbol{B} = 0, \qquad \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}, \qquad \nabla \times \boldsymbol{B} = \mu_0 \boldsymbol{J} + \mu_0 \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t}. \tag{2.1}$$

All quantities here $\boldsymbol{E}, \boldsymbol{B}, \boldsymbol{J}, \rho$ are functions of the three-dimensional position vector

$$\boldsymbol{r} = x\tilde{\boldsymbol{x}} + y\tilde{\boldsymbol{y}} + z\tilde{\boldsymbol{z}} \tag{2.2}$$

and a time variable $t \in \mathbb{R}$, where $(x, y, z) \in \mathbb{R}^3$ are the three Cartesian coordinates and

$$\{\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}, \tilde{\boldsymbol{z}}\} \tag{2.3}$$

are unit vectors in three orthogonal directions. The electric field $\boldsymbol{E}(\boldsymbol{r}, t)$, the magnetic field $\boldsymbol{B}(\boldsymbol{r}, t)$, and the current density $\boldsymbol{J}(\boldsymbol{r}, t)$ are vector fields, i.e., each vector field prescribes a three-dimensional vector at each point $(\boldsymbol{r}, t)$ in space and time, while the charge density $\rho(\boldsymbol{r}, t)$ is a scalar field, i.e., it prescribes a real number at each $(\boldsymbol{r}, t)$. ϵ_0, a real positive constant, is called the free-space permittivity, and μ_0, also a real positive constant, is called the free-space permeability.

Classical EM works fantastically well except for one "tiny" problem: in the study of blackbody radiation, the physics doesn't seem right unless we assume that the energy of an EM **mode** can exist only in discrete quanta:

$$\boxed{\text{Energy in a mode} = nh\nu, \quad n = 0, 1, 2, \ldots} \tag{2.4}$$

where ν is the frequency of the EM mode in Hertz, h is the Planck constant given by

$$\boxed{h = 6.626 \cdots \times 10^{-34} \text{ Joule sec.}} \tag{2.5}$$

and n is a nonnegative integer. This is disturbing because nowhere in classical EM says that energy has to be discrete.

2.2. Sinusoidal modes of free EM fields

Before we go into quantum, we need to learn the concept of modes in classical EM. Modes are the fundamental **degrees of freedom** in EM. Each mode has a specific solution for its EM fields, and an arbitrary solution can be expressed as a linear combination of the mode fields.

To be concrete, we begin by assuming that there are no sources ($\rho = 0$, $\boldsymbol{J} = 0$), so only EM fields in free space are present. They should obey the source-free Maxwell equations

$$\nabla \cdot \boldsymbol{E} = 0, \qquad \nabla \cdot \boldsymbol{B} = 0, \qquad \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}, \qquad \nabla \times \boldsymbol{B} = \frac{1}{c^2} \frac{\partial \boldsymbol{E}}{\partial t}, \tag{2.6}$$

where

$$c \equiv \frac{1}{\sqrt{\mu_0 \epsilon_0}} \approx 3 \times 10^8 \text{ m/s} \tag{2.7}$$

is the speed of light. Think of the dynamics as an initial-value problem: given some EM fields at $t = 0$, what are the fields at a later time t?

There are a few other assumptions we can make to simplify the math: consider EM fields in a **box**, each side with length L, and periodic boundary conditions on all sides of the box. In other words, we assume

$$x \in \left[-\frac{L}{2}, \frac{L}{2}\right], \qquad y \in \left[-\frac{L}{2}, \frac{L}{2}\right], \qquad z \in \left[-\frac{L}{2}, \frac{L}{2}\right], \tag{2.8}$$

and the EM fields at $x = -L/2$ are equal to the fields at $x = L/2$, the fields at $y = -L/2$ are equal to the fields at $y = L/2$, etc. To model EM fields in infinite space, we'd take the limit $L \to \infty$, but we won't do that for now to simplify the math.

The periodic boundary condition doesn't sound physical, but it simplifies the math and we care about the solution only as an approximation of $L \to \infty$ anyway, when the boundary condition shouldn't matter. If you want, you can assume other boundary conditions, e.g., the walls of the box are perfect conductors; the result will be the same in the $L \to \infty$ limit.

One approach of solving the Maxwell's equations in free space that will also work in quantum optics is to write the fields at initial time $t = 0$ as

$$\boldsymbol{E}(\boldsymbol{r}, 0) = \sum_j \left[\alpha_j \boldsymbol{u}_j(\boldsymbol{r}) + \alpha_j^* \boldsymbol{u}_j^*(\boldsymbol{r})\right], \tag{2.9}$$

$$\boldsymbol{B}(\boldsymbol{r}, 0) = \sum_j \frac{1}{\omega_j} \boldsymbol{k} \times \left[\alpha_j \boldsymbol{u}_j(\boldsymbol{r}) + \alpha_j^* \boldsymbol{u}_j^*(\boldsymbol{r})\right]. \tag{2.10}$$

A simpler way of writing these expressions is

$$\boldsymbol{E}(\boldsymbol{r}, 0) = \sum_j \left[\alpha_j \boldsymbol{u}_j(\boldsymbol{r}) + \text{c.c.}\right], \tag{2.11}$$

$$\boldsymbol{B}(\boldsymbol{r}, 0) = \sum_j \frac{1}{\omega_j} \boldsymbol{k} \times \left[\alpha_j \boldsymbol{u}_j(\boldsymbol{r}) + \text{c.c.}\right]. \tag{2.12}$$

where c.c. denotes the complex conjugate of the first term in the square bracket. Each term in the sum is the E field or the B field of a mode, labeled by the mode index j. Let's examine the expressions in detail:

(1) The central quantity in these expansions is the **mode function** $\boldsymbol{u}_j(\boldsymbol{r})$. It is a complex vector field given by

$$\boxed{\boldsymbol{u}_j(\boldsymbol{r}) = \frac{1}{L^{3/2}} \tilde{\boldsymbol{e}}_j \exp(i\boldsymbol{k} \cdot \boldsymbol{r}).} \tag{2.13}$$

This corresponds to a complex **sinusoidal wave** in EM. Each sinusoidal wave is a mode.

Remark 2.1. *In both classical and quantum optics, it is extremely convenient, and indeed standard, to* ***regard the electric field as complex, i.e., we omit the complex conjugate (c.c.) in a lot of discussions of the electric field.*** *If you see a complex electric field in any discussion, just assume that the electric field in reality is the complex solution + c.c.*

(2) Each **mode index** j of the mode function $\boldsymbol{u}_j(\boldsymbol{r})$ is really a shorthand for a set of quantities

$$\boxed{j = (\boldsymbol{k}, s)} \tag{2.14}$$

that specify the mode, where

$$\boxed{\boldsymbol{k} = k_x \tilde{\boldsymbol{x}} + k_y \tilde{\boldsymbol{y}} + k_z \tilde{\boldsymbol{z}}} \tag{2.15}$$

is a real vector called the **wavevector** of the mode. The length of $\boldsymbol{k}$, denoted as $|\boldsymbol{k}|$ or k, is the wavenumber given by

$$\boxed{k \equiv |\boldsymbol{k}| = \sqrt{k_x^2 + k_y^2 + k_z^2}.} \tag{2.16}$$

Define the unit vector of $\boldsymbol{k}$ as

$$\tilde{\boldsymbol{k}} \equiv \frac{\boldsymbol{k}}{k}, \tag{2.17}$$

and assume that it is one of the three axes of another Cartesian coordinate system. Let $\tilde{\boldsymbol{e}}_1$ and $\tilde{\boldsymbol{e}}_2$ be the other unit vectors for the other two axes; see Fig. 2.1. **Then $\tilde{\boldsymbol{k}} \cdot \boldsymbol{r}$ is the coordinate of $\boldsymbol{r}$ along the $\tilde{\boldsymbol{k}}$ axis**, $\tilde{\boldsymbol{e}}_1 \cdot \boldsymbol{r}$ is the coordinate of $\boldsymbol{r}$ along the $\tilde{\boldsymbol{e}}_1$ axis, etc. we can write $\boldsymbol{r}$ as

$$\boldsymbol{r} = (\tilde{\boldsymbol{k}} \cdot \boldsymbol{r})\tilde{\boldsymbol{k}} + (\tilde{\boldsymbol{e}}_1 \cdot \boldsymbol{r})\tilde{\boldsymbol{e}}_1 + (\tilde{\boldsymbol{e}}_2 \cdot \boldsymbol{r})\tilde{\boldsymbol{e}}_2. \tag{2.18}$$

The sinusoidal function $\exp(i\boldsymbol{k} \cdot \boldsymbol{r}) = \exp\Big[ik(\tilde{\boldsymbol{k}} \cdot \boldsymbol{r})\Big]$ is **periodic** with respect to the coordinate $\tilde{\boldsymbol{k}} \cdot \boldsymbol{r}$ along the $\tilde{\boldsymbol{k}}$ axis but doesn't depend on the other two coordinates. This means that if we look at any point in space and move in any direction along $\tilde{\boldsymbol{e}}_1$ or $\tilde{\boldsymbol{e}}_2$, the function stays constant in the plane perpendicular to $\boldsymbol{k}$. A sinusoidal wave is thus an example of a plane wave.

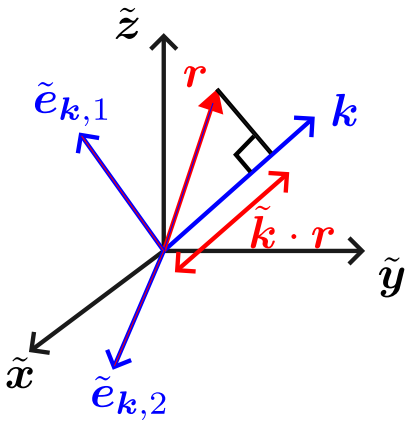

FIGURE 2.1. Let $\tilde{\boldsymbol{k}} \equiv \boldsymbol{k}/|\boldsymbol{k}|$ be the unit vector pointing in the direction of $\boldsymbol{k}$. We can write $\boldsymbol{k} \cdot \boldsymbol{r} = k(\tilde{\boldsymbol{k}} \cdot \boldsymbol{r})$. When we take the dot product of the position vector $\boldsymbol{r}$ with a unit vector $\tilde{\boldsymbol{k}}$, $\tilde{\boldsymbol{k}} \cdot \boldsymbol{r}$ is the **coordinate** of the position $\boldsymbol{r}$ along the $\boldsymbol{k}$ axis. In other words, $\exp(i\boldsymbol{k} \cdot \boldsymbol{r})$ depends on only the position coordinate along the $\boldsymbol{k}$ axis. If we think of $\tilde{\boldsymbol{k}}$ as one of the three axes of another Cartesian coordinate system, then $\exp(i\boldsymbol{k} \cdot \boldsymbol{r})$ does not depend on the other coordinates along the other directions $\tilde{\boldsymbol{e}}_{\boldsymbol{k},1}$ and $\tilde{\boldsymbol{e}}_{\boldsymbol{k},2}$. For example, if $\boldsymbol{k} = k\tilde{\boldsymbol{z}}$, then $\exp(i\boldsymbol{k} \cdot \boldsymbol{r}) = \exp(ikz)$ is periodic with respect to the z coordinate but stays constant along x and y.

Only sinusoids with certain discrete values of the wavevector can satisfy the periodic boundary conditions. To be specific, each wavevector has three real components chosen from the following possible values

$$k_x = \frac{2\pi n_x}{L}, \qquad k_y = \frac{2\pi n_y}{L}, \qquad k_z = \frac{2\pi n_z}{L}, \qquad n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots \tag{2.19}$$

It is often useful to denote each wavevector of a mode as a point in $\boldsymbol{k}$ space, as shown in Fig. 2.2. If we assume an infinitely big box $L \to \infty$, then the three components would become three continuous real variables, i.e., $(k_x, k_y, k_z) \in \mathbb{R}^3$, and $\boldsymbol{k}$ can be an arbitrary real vector.

(3) The second quantity s in the mode index $j = (\boldsymbol{k}, s)$ denotes the **polarization** of the mode. There are two possible values for s and we usually write

$$s \in \{1, 2\}, \tag{2.20}$$

denoting the two possible polarizations of each sinusoidal wave given a wavevector $\boldsymbol{k}$. $\tilde{\boldsymbol{e}}_j = \tilde{\boldsymbol{e}}_{\boldsymbol{k},s}$ is the **unit polarization vector** of the mode—$\tilde{\boldsymbol{e}}_{\boldsymbol{k},1}$ is one polarization vector and $\tilde{\boldsymbol{e}}_{\boldsymbol{k},2}$ is the other polarization

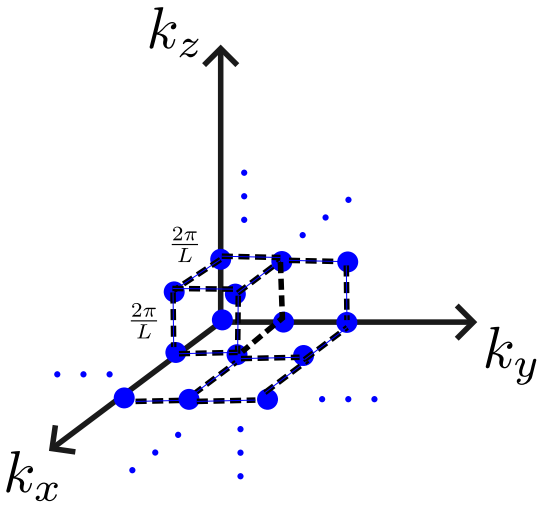

FIGURE 2.2. Each dot denotes a possible wavevector $\boldsymbol{k}$ of an EM mode inside a box with lengths all equal to L. The set of all wavevectors form a rectangular lattice in $\boldsymbol{k}$ space. Two adjacent wavevectors are separated by a distance of $2\pi/L$.

vector. We can write it as

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},s} = e_x \tilde{\boldsymbol{x}} + e_y \tilde{\boldsymbol{y}} + e_z \tilde{\boldsymbol{z}} \tag{2.21}$$

where e_x, e_y, e_z are complex numbers that are also functions of $(\boldsymbol{k}, s)$. They may be complex numbers in case we want to assume circular polarizations. Often it is too tedious to write down $\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}$ explicitly and it suffices to know that it obeys the properties

$$\boldsymbol{k} \cdot \tilde{\boldsymbol{e}}_{\boldsymbol{k},s} = 0 \qquad \text{(polarization is perpendicular to wavevector)} \tag{2.22}$$

$$\tilde{\boldsymbol{e}}^*_{\boldsymbol{k},s} \cdot \tilde{\boldsymbol{e}}_{\boldsymbol{k},s'} = \delta_{ss'} \equiv \begin{cases} 1, & s = s' \\ 0, & s \neq s' \end{cases} \qquad \text{(unit length, orthogonal polarizations)} \tag{2.23}$$

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},1} \times \tilde{\boldsymbol{e}}_{\boldsymbol{k},2} = \tilde{\boldsymbol{k}}. \qquad \text{(right-hand rule for } \tilde{\boldsymbol{e}}_{\boldsymbol{k},1}, \tilde{\boldsymbol{e}}_{\boldsymbol{k},2}, \tilde{\boldsymbol{k}}) \tag{2.24}$$

δ is called the **Kronecker delta**. The complex conjugate $*$ operation on a vector $\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}$ means that we take the complex conjugate of each of its Cartesian components.

(4) The sum $\sum_j$ is really $\sum_{\boldsymbol{k}} \sum_s$, i.e., we sum over all possible values of the wavevector $\boldsymbol{k}$ of the modes according to Eq. (2.19) and all possible polarizations s of the modes according to Eq. (2.20).

(5) ω_j is the **natural frequency** of the mode j (angular, with the unit radian/sec). It is a function of the wavevector $\boldsymbol{k}$ only and given by

$$\omega_j = c|\boldsymbol{k}|, \tag{2.25}$$

where c is the speed of light given by Eq. (2.7).

(6) The mode functions here are **orthonormal**, in the sense that

$$\iiint_{\text{box}} \boldsymbol{u}^*_j(\boldsymbol{r}) \cdot \boldsymbol{u}_l(\boldsymbol{r}) d^3\boldsymbol{r} = \delta_{jl} \equiv \begin{cases} 1, & j = l, \\ 0, & j \neq l. \end{cases} \tag{2.26}$$

The operation on the left-hand side is called an **inner product** between two vectoral functions $\boldsymbol{u}_j(\boldsymbol{r})$ and $\boldsymbol{u}_l(\boldsymbol{r})$. The integral is over the whole 3D space of the box. The Kronecker delta means that, if we take the inner product of a mode function with itself, we get 1 (i.e., the mode function is normalized), and if we take the inner product of one mode function with another mode function, we get 0 (i.e., the mode functions are "orthogonal" to one another).

(7) Each α_j is a complex number that we call the **amplitude** of mode j. The amplitudes are determined by the initial conditions, such as $\boldsymbol{E}(\boldsymbol{r},0)$ and $\frac{\partial \boldsymbol{E}(\boldsymbol{r},t)}{\partial t}\Big|_{t=0}$, although we won't need to know how exactly.

In principle, if an experimenter has total control of the initial conditions, they will be free to set the amplitude α_j of each mode to be an arbitrary complex number. This is why we call each mode a degree of freedom: its initial condition in terms of α_j can be arbitrary and is not required to depend on the initial conditions of other modes. (A proof of this fact is too tedious and we take it as given here.)

Side note. *You may think of the mode functions as a basis for the fields, i.e., any EM fields can be expressed as a linear combination of the mode functions, and the algebra of vector fields, e.g., inner product, is very similar to the linear algebra described in Appendix B, even though we are still working with classical physics.*

Here's the neat thing about Eqs. (2.11) and (2.12): once we've found the amplitudes $\{\alpha_j\}$ from the initial conditions, the fields at a later time t are simply given by

$$\boxed{\boldsymbol{E}(\boldsymbol{r},t) = \sum_j [\alpha_j \exp(-i\omega_j t)\boldsymbol{u}_j(\boldsymbol{r}) + \text{c.c.}].} \tag{2.27}$$

$$\boxed{\boldsymbol{B}(\boldsymbol{r},t) = \sum_j \frac{1}{\omega_j}\boldsymbol{k} \times [\alpha_j \exp(-i\omega_j t)\boldsymbol{u}_j(\boldsymbol{r}) + \text{c.c.}],} \tag{2.28}$$

Everything looks exactly the same as Eqs. (2.11) and (2.12), except that **we multiply each mode amplitude by** $\exp(-i\omega_j t)$. Each mode of the EM fields has a very simple time dependence: it simply oscillates at the natural frequency $\omega_j = c|\boldsymbol{k}|$. When the modes have this simple time dependence, we call the modes **the normal modes** of the fields.

Remark 2.2. *The word "normal" is definitely way overused in physics and mathematics. It means different things in different contexts, so be careful.*

You can check that Eqs. (2.27) and (2.28) satisfy the source-free Maxwell's equations at all times. Notice also that

$$\alpha_j \exp(-i\omega_j t)\boldsymbol{u}_j(\boldsymbol{r}) \propto \tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\alpha_j \exp(i\boldsymbol{k}\cdot\boldsymbol{r} - ic|\boldsymbol{k}|t), \tag{2.29}$$

which is the sinusoidal plane-wave solution of EM fields that we know and love. α_j is the complex amplitude of the wave; it tells us how strong each sinusoidal wave is (via its magnitude $|\alpha_j|$) and also the phase of the wave (via its phase $\angle\alpha_j$).

2.3. Energy of EM modes

Another neat thing about the normal-mode expansion of the EM fields is that the total energy at any given time becomes very simple:

$$\boxed{\text{total energy} = 2\epsilon_0 \sum_j |\alpha_j|^2,} \tag{2.30}$$

where ϵ_0 is the free-space permittivity. Each mode has energy

$$\boxed{\text{energy in mode } j = 2\epsilon_0 |\alpha_j|^2,} \tag{2.31}$$

and the total energy is simply the sum of all the energies of all the modes. Remember α_j is any complex number, so $|\alpha_j|^2$ can be any nonnegative number, and the energy of each mode can be any nonnegative number in classical EM.

2.4. Each normal mode is a harmonic oscillator

We now come to a crucial viewpoint that will help us quantize EM fields: Think of each normal mode as a harmonic oscillator. Remember that α_j is a complex amplitude that models the oscillation of each normal mode. As a function of time t, the complex amplitude for each mode is simply

$$\alpha_j(t) = \alpha_j \exp(-i\omega_j t). \tag{2.32}$$

Define the "position" variable as

$$q_j(t) \equiv \frac{1}{\sqrt{2}}\big[\alpha_j(t) + \alpha_j^*(t)\big], \tag{2.33}$$

and the "momentum" variable as

$$p_j(t) = \frac{1}{\sqrt{2}i}\big[\alpha_j(t) - \alpha_j^*(t)\big]. \tag{2.34}$$

Then we find that

$$\frac{dq_j(t)}{dt} = \omega_j p_j(t), \qquad \frac{dp_j(t)}{dt} = -\omega_j q_j(t), \tag{2.35}$$

$$q_j(t) = q_j(0)\cos(\omega_j t) + p_j(0)\sin(\omega_j t), \qquad p_j(t) = -q_j(0)\sin(\omega_j t) + p_j(0)\cos(\omega_j t). \tag{2.36}$$

These are the same as the equations of motion for a harmonic oscillator with natural frequency ω_j. Moreover, notice that each normal mode is, by definition, **uncoupled** to the other normal modes: the equations of motion for each normal mode depend only on the variables of that mode, and any motion of the other modes does not bother it at all.

Remark 2.3. *Other problems, e.g., in mechanics, may define the "position" and "momentum" variables differently with different constants in front, but we can always get the versions here by a simple rescaling.*

A useful picture of the harmonic-oscillator dynamics in a **phase space** is shown in Fig. 2.3. In EM and optics, the $q_j(t)$ and $p_j(t)$ variables are also called **quadratures**. We will call $q_j(t)$ the **q-quadrature** and $p_j(t)$ the **p-quadrature** to avoid confusion with the position vector $\boldsymbol{r}$ and the wavevector $\boldsymbol{k}$, which are apples and oranges.

Remark 2.4. *It is important to stress that the quadratures here determine the oscillations of the EM fields in each mode; they are not the position and momentum of any object moving in real space. $q_j(t)$ and $p_j(t)$ merely behave like position and momentum mathematically; they are called* generalized *coordinates in Hamiltonian mechanics.*

Side note. *The terminology "quadratures" comes from communication theory (https://en.wikipedia.org/wiki/Quadrature_amplitude_modulation).*

A strategy of quantizing the EM fields is now at hand: assume that each normal mode is a quantum harmonic oscillator, and the real and imaginary parts of the complex amplitude become "position" and "momentum" operators. This is indeed what Dirac did when he wrote down the first fully quantum theory of EM [4].

Most importantly, we know that the energy of a quantum harmonic oscillator is **quantized**, so we are able to prove the quantization of the EM energy of each mode using Dirac's theory.

With the concept of normal modes, we can already derive the spectrum of blackbody radiation following Planck; see Appendix A.

Exercise 2.1. Verify Eq. (2.26).

Exercise 2.2. What is the wavelength of each sinusoidal mode, given $\boldsymbol{k}$? How is it related to ω_j and the frequency in Hertz $\nu_j \equiv \omega_j/(2\pi)$?

Exercise 2.3. Check that $\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$ satisfies the periodic boundary condition along x, y, z.

Exercise 2.4. Suppose that we write the wavevector $\boldsymbol{k}$ in the spherical coordinate system as

$$\boldsymbol{k} = k(\sin\theta\cos\phi\tilde{\boldsymbol{x}} + \sin\theta\sin\phi\tilde{\boldsymbol{y}} + \cos\theta\tilde{\boldsymbol{z}}). \tag{2.37}$$

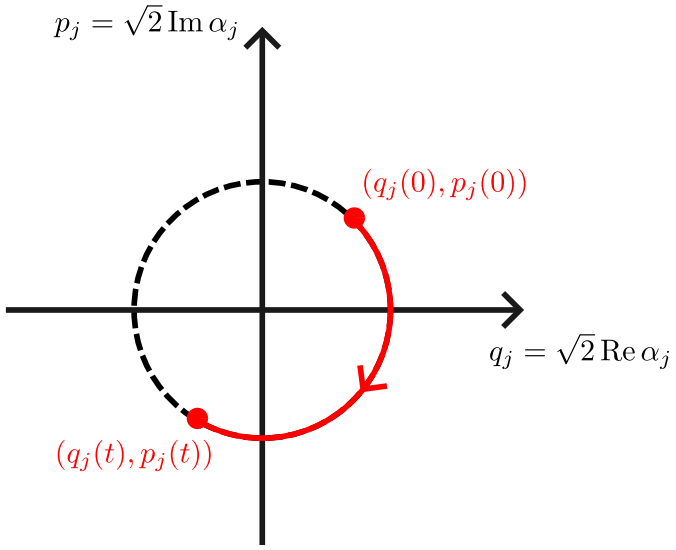

FIGURE 2.3. In the phase space, we think of the q-quadrature q_j and the p-quadrature p_j as two orthogonal axes. It's useful to visualize $(q_j(t), p_j(t))$ as a phase-space trajectory. For a harmonic oscillator, the trajectory is a clockwise circular path.

Show that

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},1} = \cos\theta\cos\phi\tilde{\boldsymbol{x}} + \cos\theta\sin\phi\tilde{\boldsymbol{y}} - \sin\theta\tilde{\boldsymbol{z}}, \tag{2.38}$$

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},2} = -\sin\phi\tilde{\boldsymbol{x}} + \cos\phi\tilde{\boldsymbol{y}} \tag{2.39}$$

satisfy Eqs. (2.22)–(2.24).

Exercise 2.5. Suppose that

$$\boldsymbol{k} = k\tilde{\boldsymbol{z}}, \qquad \tilde{\boldsymbol{e}}_{\boldsymbol{k},1} = \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}} + i\tilde{\boldsymbol{y}}). \tag{2.40}$$

Find $\tilde{\boldsymbol{e}}_{\boldsymbol{k},2}$ so that Eqs. (2.22)–(2.24) are satisfied. If the electric field at a certain position is given by

$$\boldsymbol{E}(0,t) \propto \tilde{\boldsymbol{e}}_{\boldsymbol{k},1}\exp(-i\omega_j t) + \tilde{\boldsymbol{e}}^*_{\boldsymbol{k},1}\exp(i\omega_j t), \tag{2.41}$$

Describe how the electric-field vector changes as a function of time. Do the same if

$$\boldsymbol{E}(0,t) \propto \tilde{\boldsymbol{e}}_{\boldsymbol{k},2}\exp(-i\omega_j t) + \tilde{\boldsymbol{e}}^*_{\boldsymbol{k},2}\exp(i\omega_j t). \tag{2.42}$$

Exercise 2.6. Using Eqs. (2.37)–(2.39), show that the following formula holds:

$$\sum_s e_u(\boldsymbol{k},s)e_v(\boldsymbol{k},s) = \delta_{uv} - \frac{k_u k_v}{k^2}, \tag{2.43}$$

where $u, v \in \{x, y, z\}$ and $e_u(\boldsymbol{k}, s)$ is the component of $\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}$ along the $\tilde{\boldsymbol{u}}$ axis. Do the same for the vectors in Exercise 2.5. Also try to derive this formula just from Eqs. (2.22)–(2.24).

Exercise 2.7. Verify that Eqs. (2.27) and (2.28) obey the source-free Maxwell's equations in free space.

Exercise 2.8. The EM energy density (energy per unit volume) is given by

$$\mathcal{E}(\boldsymbol{r},t) = \frac{\epsilon_0}{2}\boldsymbol{E}(\boldsymbol{r},t)\cdot\boldsymbol{E}(\boldsymbol{r},t) + \frac{1}{2\mu_0}\boldsymbol{B}(\boldsymbol{r},t)\cdot\boldsymbol{B}(\boldsymbol{r},t). \tag{2.44}$$

Use this equation and Eqs. (2.27) and (2.28) to verify Eq. (2.30).

CHAPTER 3

Quantization of Free EM Fields

Chapter 2 shows that there are many normal modes for EM fields in a box. Each mode is labeled by

$$j = (\boldsymbol{k}, s) \tag{3.1}$$

in terms of the wavevector $\boldsymbol{k}$ and the polarization s. Each mode oscillates in time at a frequency

$$\omega_j = c|\boldsymbol{k}|, \tag{3.2}$$

and the equations of motion for each mode are uncoupled from those of all other modes. These facts are hints that we may treat each mode as a **quantum harmonic oscillator**. Simply put, quantum EM is nothing but **a large number of quantum harmonic oscillators**.

We will be using the abstract Hilbert-space theory with the bra-ket notation, as reviewed in Appendix B.

3.1. Quantum harmonic oscillator

Let us focus on just **one mode** for now and review the theory of one quantum harmonic oscillator using the language of quantum optics. We begin by assuming that the Hilbert space $\mathcal{H}$ possesses an orthonormal basis

$$\{|n\rangle : n \in \{0, 1, 2, \dots\}\} \tag{3.3}$$

where each $|n\rangle$ models the state of the mode with an integer photon number $n \in \{0, 1, 2, \dots\}$. We call each $|n\rangle$ a **number state**. The number states are orthonormal in the sense that

$$\langle n|m\rangle = \delta_{nm} \equiv \begin{cases} 1, & n = m, \\ 0, & n \neq m. \end{cases} \tag{3.4}$$

To express the fact that the number states are a basis of the Hilbert space, we use the **completeness condition**

$$\boxed{\hat{I} = \sum_{n=0}^{\infty} |n\rangle \langle n|,} \tag{3.5}$$

where $\hat{I}$ is the identity operator, defined by $\hat{I}|\psi\rangle = |\psi\rangle$ for any $|\psi\rangle \in \mathcal{H}$. This relation says that any $|\psi\rangle$ can be written as

$$|\psi\rangle = \hat{I}|\psi\rangle = \sum_{n=0}^{\infty} |n\rangle \langle n|\psi\rangle, \tag{3.6}$$

which is a linear combination of $\{|n\rangle\}$. Orthonormality + completeness together imply that the set $\{|n\rangle\}$ is an orthonormal basis.

Any quantum state can be expressed as a superposition of the number states:

$$|\psi\rangle = \sum_{n=0}^{\infty} \psi_n |n\rangle, \tag{3.7}$$

where $\psi_n = \langle n|\psi\rangle$ as a function of n is the wavefunction in the number basis. If the state is normalized, we assume

$$\langle\psi|\psi\rangle = 1. \tag{3.8}$$

This implies that the wavefunction should also be normalized as

$$\sum_{n=0}^{\infty} |\psi_n|^2 = 1. \tag{3.9}$$

Define an **annihilation** operator $\hat{a}$ and a **creation** operator $\hat{a}^\dagger$, which is the adjoint of $\hat{a}$. They are so called because the effect of applying $\hat{a}$ on each number state is to reduce the number as follows:

$$\boxed{\hat{a}\,|0\rangle = 0,} \qquad \boxed{\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \quad n = 1, 2, \ldots} \tag{3.10}$$

while the effect of applying $\hat{a}^\dagger$ on each number state is to increase the number as follows:

$$\boxed{\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,.} \tag{3.11}$$

The annihilation and creation operators satisfy the commutation relation

$$\boxed{\left[\hat{a}, \hat{a}^\dagger\right] = \hat{I}.} \tag{3.12}$$

The number operator is defined as

$$\boxed{\hat{n} \equiv \hat{a}^\dagger \hat{a},} \tag{3.13}$$

and each number state is an eigenstate of $\hat{n}$, with eigenvalue n:

$$\boxed{\hat{n}\,|n\rangle = n\,|n\rangle\,.} \tag{3.14}$$

We can then write $\hat{n}$ in the diagonal form

$$\boxed{\hat{n} = \sum_{n=0}^{\infty} n\,|n\rangle\,\langle n|\,.} \tag{3.15}$$

To represent the quadratures of the mode, we define the Hermitian operators

$$\boxed{\hat{q} \equiv \frac{1}{\sqrt{2}}\left(\hat{a} + \hat{a}^\dagger\right),} \tag{3.16}$$

$$\boxed{\hat{p} \equiv \frac{1}{\sqrt{2}i}\left(\hat{a} - \hat{a}^\dagger\right).} \tag{3.17}$$

Mathematically, these really behave like the position and momentum operators we know and love in elementary quantum mechanics; different people may put different constants in front of these formulas but we'll stick to our definition here.

Our quadrature operators obey the commutation relation

$$\boxed{[\hat{q}, \hat{p}] = i\hat{I}.} \tag{3.18}$$

We often write

$$\boxed{[\hat{a}, \hat{a}^\dagger] = 1,} \qquad \boxed{[\hat{q}, \hat{p}] = i,} \tag{3.19}$$

by replacing $\hat{I}$ with 1. This is slightly sloppy, since a commutator of two operators is supposed to give another operator, but it is a harmless abbreviation since $\hat{I}$ and 1 act on everything in exactly the same way.

Another basis of the Hilbert space can be constructed from the q-quadrature eigenstates

$$\{|q = x\rangle : x \in \mathbb{R}\}. \tag{3.20}$$

They are defined by

$$\boxed{\hat{q}\,|q=x\rangle = x\,|q=x\rangle\,,} \tag{3.21}$$

$$\boxed{\langle q=x|q=x'\rangle = \delta(x-x'),} \tag{3.22}$$

such that the diagonal form of $\hat{q}$ is

$$\boxed{\hat{q} = \int_{-\infty}^{\infty} x\,|q=x\rangle\,\langle q=x|\,dx,} \tag{3.23}$$

and the completeness condition is

$$\boxed{\hat{I} = \int_{-\infty}^{\infty} |q=x\rangle\,\langle q=x|\,dx.} \tag{3.24}$$

Similarly, for the p-quadrature operator $\hat{p}$,

$$\boxed{\hat{p}\,|p=y\rangle = y\,|p=y\rangle\,,} \qquad \boxed{\langle p=y|p=y'\rangle = \delta(y-y'),} \tag{3.25}$$

$$\boxed{\hat{p} = \int_{-\infty}^{\infty} y\,|p=y\rangle\,\langle p=y|\,dy,} \qquad \boxed{\hat{I} = \int_{-\infty}^{\infty} |p=y\rangle\,\langle p=y|\,dy.} \tag{3.26}$$

Remark 3.1. *Do not confuse the x, y here (eigenvalue of $|q=x\rangle$ or $|p=y\rangle$) with the coordinates of the position vector $\boldsymbol{r} = x\tilde{\boldsymbol{x}} + y\tilde{\boldsymbol{y}} + z\tilde{\boldsymbol{z}}$! They are completely unrelated things. Unfortunately we have to recycle symbols for different uses a lot, as is often the case in physics.*

To relate the two sets of eigenstates, we have the following relations

$$\boxed{\langle q=x|p=y\rangle = \frac{1}{\sqrt{2\pi}}\exp(iyx),} \tag{3.27}$$

$$\boxed{|p=y\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp(iyx)\,|q=x\rangle\,dx,} \tag{3.28}$$

$$\boxed{|q=x\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp(-iyx)\,|p=y\rangle\,dy.} \tag{3.29}$$

The preceding discussion can be applied to a lot of quantum systems with infinite-dimensional Hilbert spaces, not just harmonic oscillators. What makes the system a harmonic oscillator is its Hamiltonian

$$\boxed{\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} = \hbar\omega\hat{n},} \tag{3.30}$$

where

(1) we have made the harmless assumption that the ground-state energy is zero,
(2)

$$\boxed{\hbar \equiv \frac{h}{2\pi}} \tag{3.31}$$

is Planck's constant divided by 2π (we'll be using $\hbar$ mostly rather than h).
(3) ω is the **natural frequency** of the mode (the frequency at which the harmonic oscillator oscillates in classical physics).

The eigenvalues of $\hat{H} = \hbar\omega\hat{n}$ are $0, \hbar\omega, 2\hbar\omega, \ldots$, and if we measure $\hat{H}$ in a von Neumann measurement, the outcome is always one of the eigenvalues. This is one key reason that we model EM fields as quantum harmonic oscillators—to make it fit with evidence from blackbody radiation that the EM energy of each mode is quantized.

Another way to see that the harmonic-oscillator model is the right one is to look at its equations of motion in the **Heisenberg picture**. Define the unitary operator

$$\hat{U}(t) \equiv \exp\left(-\frac{i}{\hbar}\hat{H}t\right). \tag{3.32}$$

The Heisenberg picture of an operator $\hat{O}$ is defined as

$$\hat{O}(t) \equiv \hat{U}^\dagger(t)\hat{O}\hat{U}(t), \tag{3.33}$$

which obeys the equation of motion

$$\frac{d\hat{O}(t)}{dt} = -\frac{i}{\hbar}\Big[\hat{O}(t), \hat{H}\Big] = -\frac{i}{\hbar}\hat{U}^\dagger(t)\Big[\hat{O}, \hat{H}\Big]\hat{U}(t). \tag{3.34}$$

Assume that $\hat{a}(0) = \hat{a}, \hat{q}(0) = \hat{q}, \hat{p}(0) = \hat{p}$ are operators at $t = 0$ in the Heisenberg picture. Define the Heisenberg-picture operators as

$$\hat{a}(t) \equiv \hat{U}^\dagger(t)\hat{a}\hat{U}(t), \qquad \hat{q}(t) \equiv \hat{U}^\dagger(t)\hat{q}\hat{U}(t), \qquad \hat{p}(t) \equiv \hat{U}^\dagger(t)\hat{p}\hat{U}(t). \tag{3.35}$$

Then it is straightforward to show that

$$\frac{d\hat{a}(t)}{dt} = -i\omega\hat{a}(t), \qquad \boxed{\hat{a}(t) = \hat{a}\exp(-i\omega t),} \tag{3.36}$$

$$\hat{q}(t) = \frac{1}{\sqrt{2}}\Big[\hat{a}(t) + \hat{a}^\dagger(t)\Big], \qquad \hat{p}(t) = \frac{1}{\sqrt{2}i}\Big[\hat{a}(t) - \hat{a}^\dagger(t)\Big], \tag{3.37}$$

$$\frac{d\hat{q}(t)}{dt} = \omega\hat{p}(t), \qquad \frac{d\hat{p}(t)}{dt} = -\omega\hat{q}(t). \tag{3.38}$$

These Heiseberg equations agree with the classical ones in Sec. 2.4.

Exercise 3.1. Derive the formulas

$$\boxed{\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p}),} \qquad \boxed{\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p}),} \tag{3.39}$$

Exercise 3.2. Prove the following:

$$\boxed{|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle.} \tag{3.40}$$

Exercise 3.3. Compute

$$\langle n|\,\hat{q}\,|n\rangle, \quad \langle n|\,\hat{p}\,|n\rangle, \quad \langle n|\,\hat{q}^2\,|n\rangle, \quad \langle n|\,\hat{p}^2\,|n\rangle, \quad \langle n|\,\hat{q}\hat{p}\,|n\rangle, \quad \langle n|\,\hat{p}\hat{q}\,|n\rangle \tag{3.41}$$

for a number state $|n\rangle$.

Exercise 3.4. The variance of a Hermitian operator $\hat{A}$ is defined as

$$\langle\Delta A^2\rangle \equiv \langle\psi|\,\hat{A}^2\,|\psi\rangle - \Big(\langle\psi|\,\hat{A}\,|\psi\rangle\Big)^2. \tag{3.42}$$

The uncertainty relation for the quadratures would then be given by

$$\langle\Delta q^2\rangle\,\langle\Delta p^2\rangle \geq C, \tag{3.43}$$

where C is a certain constant. Use the uncertainty relation you learned from quantum mechanics to find C. Compute $\langle\Delta q^2\rangle$ and $\langle\Delta p^2\rangle$ for a number state $|n\rangle$ and confirm that the uncertainty relation is satisfied.

Exercise 3.5. Define the Heisenberg picture of annihilation and creation operators as

$$\hat{a}(t) \equiv \hat{U}^\dagger(t)\hat{a}\hat{U}(t), \qquad \hat{a}^\dagger(t) \equiv \hat{U}^\dagger(t)\hat{a}^\dagger\hat{U}(t), \tag{3.44}$$

where $\hat{U}$ is an arbitrary unitary operator (not necessarily that for a harmonic oscillator). Prove that the equal-time commutation relation remains

$$\boxed{\left[\hat{a}(t), \hat{a}^\dagger(t)\right] = \hat{I}.} \tag{3.45}$$

(This fact is important, as it means that, even if we change the Hamiltonian to model more complicated light-matter interactions, this commutation relation must remain the same at all times in the Heisenberg picture. If your calculation violates this relation somehow, it's wrong.)

Exercise 3.6. Write the ket-bra form of $\hat{a}$ with respect to the number basis $\{|n\rangle : n = 0, 1, \dots\}$, i.e., write

$$\hat{a} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} a_{nm} |n\rangle \langle m| \tag{3.46}$$

and find the matrix entries a_{nm}. Do the same for $\hat{a}^\dagger$, $\hat{q}$, and $\hat{p}$.

Exercise 3.7. Numerical exercise: The matrix representation of $\hat{q}$ with respect to the number basis has infinite entries. Approximate $\hat{q}$ by the finite sum

$$\hat{q} \approx \sum_{n=0}^{N-1}\sum_{m=0}^{N-1} q_{nm} |n\rangle \langle m| \tag{3.47}$$

and find the eigenvalues of the right-hand side for $N = 5, 10, 20, \dots$ using a numerical software. Are they all real? How do they behave when you increase N?

Exercise 3.8. Define the q-quadrature wavefunction as

$$\psi_q(x) \equiv \langle q = x|\psi\rangle \tag{3.48}$$

and the p-quadrature wavefunction as

$$\psi_p(y) \equiv \langle p = y|\psi\rangle\,. \tag{3.49}$$

(1) Find the normalization conditions for the wavefunctions.
(2) Find the relation between the two wavefunctions.

3.2. Quantization of multiple normal modes

Now we take all the normal modes discussed in Chapter 2 and assume that each normal mode is a quantum harmonic oscillator. Recall that each normal mode is labeled by $j = (\boldsymbol{k}, s)$, and we denote the Hilbert space for the normal mode j as $\mathcal{H}_j$. We set the Hilbert space for all the normal modes to be the tensor product (see Sec. B.8) of all the individual $\mathcal{H}_j$'s, in accordance with how multiple degrees of freedom are treated in quantum mechanics.

Strictly speaking, we have an infinite number of normal modes, but I will assume for now that there are only J normal modes so that the math looks less scary. To simplify the notation even more, I will denote the J normal modes by $j = 1, 2, \dots, J$. When I write $j = 1$ I mean it's the first normal mode, and when I write $j = 2$ I mean it's the second normal mode, etc., and we don't worry about the $(\boldsymbol{k}, s)$ properties of the modes for now.

We write the Hilbert space for the J harmonic oscillators as the tensor product

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_J. \tag{3.50}$$

The important property of this big Hilbert space is that it has an orthonormal basis constructed by the number states for each $\mathcal{H}_j$:

$$\boxed{|n_1, n_2, \dots, n_J\rangle \equiv |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_J\rangle\,, \quad \text{each } n_j = 0, 1, 2, \dots} \tag{3.51}$$

In other words, $|n_1, n_2, n_3, \ldots\rangle$ denotes the quantum state with n_1 photons in mode 1, n_2 photons in mode 2, etc. Each state in $\mathcal{H}$ in general can be expressed as the superposition

$$|\psi\rangle = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_J=0}^{\infty}\psi_{n_1 n_2 \ldots n_J}\,|n_1, n_2, \ldots, n_J\rangle\,, \tag{3.52}$$

$$\psi_{n_1 n_2 \ldots n_J} = \langle n_1, n_2, \ldots, n_J|\psi\rangle\,. \tag{3.53}$$

Note that each sum $\sum_{n_j=0}^{\infty}$ is an infinite sum, and there are J such sums. The wavefunction $\psi_{n_1 \ldots n_J}$ now depends on J photon-number variables $(n_1, \ldots, n_J)$.

We can write the annihilation operator for mode j as $\hat{a}_j$. It is now defined by

$$\hat{a}_j\,|\ldots, n_{j-1}, 0, n_{j+1}, \ldots\rangle = 0, \tag{3.54}$$

$$\hat{a}_j\,|\ldots, n_{j-1}, n_j, n_{j+1}, \ldots\rangle = \sqrt{n_j}\,|\ldots, n_{j-1}, n_j - 1, n_{j+1}\ldots\rangle\,. \tag{3.55}$$

In other words, it acts on mode j in the same way as before, while leaving all the other modes alone. Mathematically, $\hat{a}_j$ is an abbreviation of

$$\hat{a}_j = \hat{I}_1 \otimes \cdots \otimes \hat{I}_{j-1} \otimes \hat{a} \otimes \hat{I}_{j+1} \otimes \cdots \otimes \hat{I}_J, \tag{3.56}$$

where each $\hat{I}_j$ is the identity operator on mode j. The identity operators do nothing to all the other modes, while $\hat{a}$ on the right-hand side acts on the Hilbert space $\mathcal{H}_j$ in the usual way.

With $\hat{a}_j$, we can now define the creation operator $\hat{a}_j^\dagger$, the photon-number operator

$$\hat{n}_j \equiv \hat{a}_j^\dagger \hat{a}_j, \tag{3.57}$$

and the quadrature operators

$$\hat{q}_j \equiv \frac{1}{\sqrt{2}}\Big(\hat{a}_j + \hat{a}_j^\dagger\Big), \qquad\qquad \hat{p}_j \equiv \frac{1}{\sqrt{2}i}\Big(\hat{a}_j - \hat{a}_j^\dagger\Big), \tag{3.58}$$

all of which act on the jth mode only and do nothing on the other modes. The important commutation relations are now given by

$$\boxed{[\hat{a}_j, \hat{a}_l] = 0,} \qquad \boxed{\left[\hat{a}_j^\dagger, \hat{a}_l^\dagger\right] = 0,} \qquad \boxed{\left[\hat{a}_j, \hat{a}_l^\dagger\right] = \delta_{jl},} \tag{3.59}$$

$$\boxed{[\hat{q}_j, \hat{q}_l] = 0,} \qquad \boxed{[\hat{p}_j, \hat{p}_l] = 0,} \qquad \boxed{[\hat{q}_j, \hat{p}_l] = i\delta_{jl}.} \tag{3.60}$$

As before, we have $[\hat{a}_j, \hat{a}_j^\dagger] = 1$ and $[\hat{q}_j, \hat{p}_j] = i$ for the same mode. The new feature here is that each operator for a mode commutes with any operator for all the other modes, so, for example, $[\hat{a}_j, \hat{a}_l^\dagger] = 0$ if $j \neq l$. Again, these definitions are pretty general for a quantum system with multiple degrees of freedom; what makes them harmonic oscillators is the Hamiltonian:

$$\boxed{\hat{H} = \sum_{j=1}^{J}\hbar\omega_j\hat{n}_j = \sum_{j=1}^{J}\hbar\omega_j\hat{a}_j^\dagger\hat{a}_j,} \tag{3.61}$$

where ω_j is the natural frequency of mode j. The Heisenberg-picture equation of motion for each mode is now given by

$$\hat{U}(t) \equiv \exp\left(-\frac{i}{\hbar}\hat{H}t\right), \qquad \frac{d\hat{a}_j(t)}{dt} = -i\omega_j\hat{a}_j(t), \qquad \boxed{\hat{a}_j(t) \equiv \hat{U}^\dagger(t)\hat{a}_j\hat{U}(t) = \hat{a}_j\exp(-i\omega_j t),} \tag{3.62}$$

which agrees with the classical version.

If your whole world consists of EM fields only, then there's nothing more you need to model it. A basic quantum-optics experiment consists of preparing some state $|\psi\rangle$ for the J normal modes at $t = 0$, let time pass, and then measure the modes—the probability distribution of the outcomes follows Born's rule. If you need to refresh your memory, probability theory is reviewed in Appendix C and quantum mechanics is reviewed in Appendix D.

Exercise 3.9. The **vacuum state** is defined as

$$\boxed{|\text{vac}\rangle \equiv |0,0,\ldots,0\rangle\,,} \tag{3.63}$$

i.e., no photon in all modes. Each number state can be written as

$$|n_1,n_2,\ldots,n_J\rangle = \hat{A}\,|\text{vac}\rangle \tag{3.64}$$

in terms of the vacuum state and a certain operator $\hat{A}$. Find $\hat{A}$.

3.3. Maxwell's equations

We still have to show that the formalism is consistent with Maxwell's equations, and the easiest way is to assume that $\hat{\boldsymbol{E}}(\boldsymbol{r},t)$ and $\hat{\boldsymbol{B}}(\boldsymbol{r},t)$ are operators in the Heisenberg picture. We replace Eqs. (2.11) and (2.12) with

$$\hat{\boldsymbol{E}}(\boldsymbol{r},0) = \sum_j \left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2}\Big[i\hat{a}_j\boldsymbol{u}_j(\boldsymbol{r}) - i\hat{a}_j^\dagger\boldsymbol{u}_j^*(\boldsymbol{r})\Big], \tag{3.65}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r},0) = \sum_j \left(\frac{\hbar}{2\epsilon_0\omega_j}\right)^{1/2}\boldsymbol{k}\times\Big[i\hat{a}_j\boldsymbol{u}_j(\boldsymbol{r}) - i\hat{a}_j^\dagger\boldsymbol{u}_j^*(\boldsymbol{r})\Big]. \tag{3.66}$$

where the complex amplitude α_j has been replaced by the annihilation operator $i\hat{a}_j$ times $(\hbar\omega_j/2\epsilon_0)^{1/2}$, while α_j^* has been replaced by $-i\hat{a}_j^\dagger$ times the same constant. The extra i is a convention that is explained in Appendix E. The factor $(\hbar\omega_j/2\epsilon_0)^{1/2}$ is introduced so that the energy of each mode computed from $\hat{\boldsymbol{E}}$ and $\hat{\boldsymbol{B}}$ becomes $\hbar\omega_j(\hat{a}_j^\dagger\hat{a}_j + 1/2)$, to make it consistent with the Hamiltonian of a harmonic oscillator. These equations are often abbreviated as

$$\hat{\boldsymbol{E}}(\boldsymbol{r},0) = \sum_j \left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2}[i\hat{a}_j\boldsymbol{u}_j(\boldsymbol{r}) + \text{H.c.}], \tag{3.67}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r},0) = \sum_j \left(\frac{\hbar}{2\epsilon_0\omega_j}\right)^{1/2}\boldsymbol{k}\times[i\hat{a}_j\boldsymbol{u}_j(\boldsymbol{r}) + \text{H.c.}], \tag{3.68}$$

where H.c. denotes the **Hermitian conjugate** (i.e., adjoint) of the first term in the square brackets.

Remark 3.2. *Beware that, on the right-hand side of Eqs. (3.67) and (3.68), $\hat{a}_j$ (and $\hat{a}_j^\dagger$ in the H.c.) are the only quantities that are operators; the rest remain c-numbers. Keep in mind that*

1. *The kets, the bras, and the operators (anything with a hat) are **abstract** quantities that we may call **Q-numbers**. Examples include $|\psi\rangle$, $\langle\psi|$, $\hat{a}_j$, and $\hat{a}_j^\dagger$. They follow the abstract Hilbert-space theory outlined in Appendix B.*
2. *Anything else without a hat is called a **c-number**. Examples include $\boldsymbol{r}$, t, $\boldsymbol{k}$, $\tilde{\boldsymbol{e}}_j$, and $\boldsymbol{u}_j(\boldsymbol{r})$. By definition, a c-number **commutes** with any Q-number, i.e., we are free to exchange the order of a Q-number and a c-number in a product.*
3. *The divergence $\nabla\cdot$, the curl $\nabla\times$, and the time derivative $\partial/\partial t$ are applied to functions of $\boldsymbol{r}$ and t in the usual sense. Do not confuse them with the abstract operators.*

For example, $\hat{a}_j$ in Eq. (3.67) is an abstract operator, and $\hat{a}_j\boldsymbol{u}_j(\boldsymbol{r})$ is simply a product of the Q-number $\hat{a}_j$ with the c-number $\boldsymbol{u}_j(\boldsymbol{r})$. If we want, we can write it as $\boldsymbol{u}_j(\boldsymbol{r})\hat{a}_j$ because they commute, and $\hat{a}_j$ is not an operator acting on $\boldsymbol{u}_j(\boldsymbol{r})$. Think of the Q-numbers as snobs that live in their own abstract world and play with themselves only; they can pass through any c-number in a product.

Now that we have clarified the algebra, it is straightforward to show that the Heisenberg equations of motion become

$$\hat{\boldsymbol{E}}(\boldsymbol{r},t) \equiv \hat{U}^\dagger(t)\hat{\boldsymbol{E}}(\boldsymbol{r},0)\hat{U}(t) = \sum_j \left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2} [i\hat{a}_j \exp(-i\omega_j t)\boldsymbol{u}_j(\boldsymbol{r}) + \text{H.c.}], \tag{3.69}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r},t) \equiv \hat{U}^\dagger(t)\hat{\boldsymbol{B}}(\boldsymbol{r},0)\hat{U}(t) = \sum_j \left(\frac{\hbar}{2\epsilon_0\omega_j}\right)^{1/2} \boldsymbol{k} \times [i\hat{a}_j \exp(-i\omega_j t)\boldsymbol{u}_j(\boldsymbol{r}) + \text{H.c.}]. \tag{3.70}$$

These operators obey the same Maxwell equations given by Eqs. (2.6) for free space with no source. They imply, for example, that, given an initial state $|\psi\rangle$, the averages

$$\langle\psi|\,\hat{\boldsymbol{E}}(\boldsymbol{r},t)\,|\psi\rangle\,, \quad \langle\psi|\,\hat{\boldsymbol{B}}(\boldsymbol{r},t)\,|\psi\rangle \tag{3.71}$$

obey Maxwell equations, so **classical EM holds on average** (you are asked to show this in Exercise 3.10). The average of a Heisenberg-picture annihilation operator

$$\langle\psi|\,\hat{a}_j \exp(-i\omega_j t)\,|\psi\rangle \tag{3.72}$$

is the average complex amplitude of mode j as it oscillates in time, and

$$\langle\psi|\,\hbar\omega_j\hat{a}_j^\dagger\hat{a}_j\,|\psi\rangle \tag{3.73}$$

is the average energy in mode j. In general, we should treat the EM variables that we measure as **random variables**, the probabilistic properties of which come from the quantum theory.

Exercise 3.10.

(1) Derive Eqs. (3.69) and (3.70) from Eqs. (3.67) and (3.68).
(2) Show that $\hat{\boldsymbol{E}}(\boldsymbol{r},t)$ and $\hat{\boldsymbol{B}}(\boldsymbol{r},t)$ obey Eqs. (2.6).
(3) Show that $\langle\psi|\,\hat{\boldsymbol{E}}(\boldsymbol{r},t)\,|\psi\rangle$ and $\langle\psi|\,\hat{\boldsymbol{B}}(\boldsymbol{r},t)\,|\psi\rangle$ obey Eqs. (2.6).

Hint: The Q-numbers $\hat{a}_j$, $\hat{a}_j^\dagger$, $|\psi\rangle$, and $\langle\psi|$ do not depend on the position vector $\boldsymbol{r}$, while $\nabla\cdot$ and $\nabla\times$ are applied to functions of $\boldsymbol{r}$.

3.4. Continuum of modes

So far we've assumed EM fields inside a box and periodic boundary conditions. This assumption is a bit artificial, and to model EM fields in infinite space, i.e., $(x,y,z) \in \mathbb{R}^3$, we should take the $L \to \infty$ limit. There are two ways of doing it: stick with the box formalism and take the $L \to \infty$ limit at the end of a calculation, or take the limit for the box formalism before starting a calculation. We will discuss the second approach in this section.

The first thing to note is that the wavevector no longer takes discrete values as per Eq. (2.19); with $L \to \infty$, $\boldsymbol{k} = k_x\tilde{\boldsymbol{x}} + k_y\tilde{\boldsymbol{y}} + k_z\tilde{\boldsymbol{z}}$ can now be an arbitrary vector, and Eq. (2.19) becomes

$$(k_x, k_y, k_z) \in \mathbb{R}^3. \tag{3.74}$$

In other words, we no longer have a discrete set of modes; we say that we have a **continuum** of modes.

Recall that the sum $\sum_j = \sum_{\boldsymbol{k}}\sum_s$ is over the discrete set of wavevectors and the two polarizations $s \in \{1,2\}$. With $(k_x,k_y,k_z) \in \mathbb{R}^3$, $\sum_{\boldsymbol{k}} = \sum_{k_x}\sum_{k_y}\sum_{k_z}$ is not really well defined, but we can turn it into an integral. To do so, we

(1) define

$$\Delta k \equiv \frac{2\pi}{L}, \tag{3.75}$$

which is the spacing between adjacent values of k_x, k_y, k_z,
(2) define a scaled annihilation operator as

$$\hat{a}(\boldsymbol{k},s) \equiv \frac{1}{\Delta k^{3/2}}\hat{a}_j, \tag{3.76}$$

(3) rewrite the mode function $\boldsymbol{u}_j(\boldsymbol{r})$ given by Eq. (2.13) as

$$\boldsymbol{u}_j(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}\left(\frac{2\pi}{L}\right)^{3/2}\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}\Delta k^{3/2}\tilde{\boldsymbol{e}}(\boldsymbol{k},s)\exp(i\boldsymbol{k}\cdot\boldsymbol{r}). \tag{3.77}$$

Then we can rewrite the electric field given by Eq. (3.67) as

$$\hat{\boldsymbol{E}}(\boldsymbol{r},0) = \frac{1}{(2\pi)^{3/2}}\sum_{k_x,k_y,k_z}\sum_s\left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2}[i\hat{a}(\boldsymbol{k},s)\tilde{\boldsymbol{e}}(\boldsymbol{k},s)\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) + \text{H.c.}]\,(\Delta k)^3. \tag{3.78}$$

Now we take the $L\to\infty$ limit, which is the same as the $\Delta k\to 0$ limit, and the triple sum $\sum_{k_x,k_y,k_z}(\dots)(\Delta k)^3$ is a Riemann sum that becomes the triple integral:

$$\boxed{\hat{\boldsymbol{E}}(\boldsymbol{r},0) = \frac{1}{(2\pi)^{3/2}}\sum_s\iiint\left(\frac{\hbar\omega_{\boldsymbol{k}}}{2\epsilon_0}\right)^{1/2}[i\hat{a}(\boldsymbol{k},s)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) + \text{H.c.}]d^3\boldsymbol{k},} \tag{3.79}$$

$$\omega_{\boldsymbol{k}} = c|\boldsymbol{k}|, \tag{3.80}$$

$$\iiint(\dots)d^3\boldsymbol{k} \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(\dots)dk_xdk_ydk_z. \tag{3.81}$$

The important new feature is that the new annihilation operator defined by Eq. (3.76) is now a function of continuous variables $(k_x,k_y,k_z)\in\mathbb{R}^3$ and obeys the commutation relation

$$\boxed{\left[\hat{a}(\boldsymbol{k},s),\hat{a}^\dagger(\boldsymbol{k}',s')\right] = \frac{1}{(\Delta k)^3}\delta_{jj'}\to\delta^3(\boldsymbol{k}-\boldsymbol{k}')\delta_{ss'},} \tag{3.82}$$

where δ^3 is the three-dimensional Dirac delta function given by

$$\delta^3(\boldsymbol{k}-\boldsymbol{k}') \equiv \delta(k_x-k_x')\delta(k_y-k_y')\delta(k_z-k_z'). \tag{3.83}$$

The magnetic field given by Eq. (3.68) likewise becomes

$$\hat{\boldsymbol{B}}(\boldsymbol{r},0) = \frac{1}{(2\pi)^{3/2}}\sum_s\iiint\left(\frac{\hbar}{2\epsilon_0\omega_{\boldsymbol{k}}}\right)^{1/2}\boldsymbol{k}\times[i\hat{a}(\boldsymbol{k},s)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) + \text{H.c.}]d^3\boldsymbol{k}. \tag{3.84}$$

In the Heisenberg picture,

$$\hat{a}(\boldsymbol{k},s,t) \equiv \hat{U}^\dagger(t)\hat{a}(\boldsymbol{k},s)\hat{U}(t) = \hat{a}(\boldsymbol{k},s)\exp(-i\omega_{\boldsymbol{k}}t), \tag{3.85}$$

and the EM fields become

$$\hat{\boldsymbol{E}}(\boldsymbol{r},t) = \frac{1}{(2\pi)^{3/2}}\sum_s\iiint\left(\frac{\hbar\omega_{\boldsymbol{k}}}{2\epsilon_0}\right)^{1/2}[i\hat{a}(\boldsymbol{k},s)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}-i\omega_{\boldsymbol{k}}t) + \text{H.c.}]d^3\boldsymbol{k}, \tag{3.86}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r},t) = \frac{1}{(2\pi)^{3/2}}\sum_s\iiint\left(\frac{\hbar}{2\epsilon_0\omega_{\boldsymbol{k}}}\right)^{1/2}\boldsymbol{k}\times[i\hat{a}(\boldsymbol{k},s)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}-i\omega_{\boldsymbol{k}}t) + \text{H.c.}]d^3\boldsymbol{k}, \tag{3.87}$$

which obey the free-space source-free Maxwell's equations, just as before.

We have succeeded in taking the $L\to\infty$ limit by using calculus. Instead of assuming a discrete set of modes, we now have a continuum of modes, where $\boldsymbol{k}$ is a vectoral continuous variable, while the polarization labeled by s remains discrete. Instead of a sum $\sum_j$ over the discrete set, we now have $\sum_s\iiint(\dots)d^3\boldsymbol{k}$, and instead of the Kronecker delta δ_{jl}, we now use $\delta^3(\boldsymbol{k}-\boldsymbol{k}')\delta_{ss'}$. We no longer need to refer to a box; L has disappeared completely from the equations. The price to pay is that the new annihilation and creation operators now obey a fancier commutation relation given by Eq. (3.82), and we don't have the simple picture of a discrete set of harmonic

oscillators anymore. For example, $\hat{a}^\dagger(\boldsymbol{k},s)\hat{a}(\boldsymbol{k},s)$ is not a photon number exactly but a photon-number density, and we get a photon-number operator only if we integrate it in $\boldsymbol{k}$-space like this:

$$\hat{n}(\mathcal{V},s)=\iiint_{\mathcal{V}}\hat{a}^\dagger(\boldsymbol{k},s)\hat{a}(\boldsymbol{k},s)d^3\boldsymbol{k}, \tag{3.88}$$

which corresponds to the total photon number in all the modes with wavevector $\boldsymbol{k}$ inside a $\boldsymbol{k}$-space volume $\mathcal{V}$. The Hilbert space in the continuum case also becomes very difficult to write down, unlike the discrete case where we have the number states $\{|n_1,\dots,n_J\rangle\}$ as an orthonormal basis. We will have to wait until Sec. 5.6 to show how.

3.5. Transformation of modes

Recall that the normal modes are sinusoidal waves. The EM fields of a sinusoidal wave remain nonzero even if we go to the ends of the universe ($x\to\pm\infty$ or $y\to\pm\infty$ or $z\to\pm\infty$), so a sinusoidal wave by itself is actually not a physical solution to Maxwell's; it is, at best, an approximation. It is thus often convenient in optics to use a different set of modes that are a bit closer to reality.

The math is simpler if we assume a discrete set of modes, so let's come back to the box formalism. The standard way of defining a different set of modes is to express the normal-mode annihilation operators $\{\hat{a}_j\}$ in terms of a new set of annihilation operators $\{\hat{b}_l\}$ as

$$\boxed{\hat{a}_j=\sum_l W_{jl}\hat{b}_l,} \tag{3.89}$$

where W is a unitary matrix with complex-number entries. To see a physical meaning of Eq. (3.89), plug it in Eq. (3.67) to obtain

$$\hat{\boldsymbol{E}}(\boldsymbol{r},0)=\sum_j\left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2}\left[i\sum_l W_{jl}\hat{b}_l\boldsymbol{u}_j(\boldsymbol{r})+\text{H.c.}\right]=\left(\frac{\hbar}{2\epsilon_0}\right)^{1/2}\sum_l\left[i\hat{b}_l\boldsymbol{v}_l(\boldsymbol{r})+\text{H.c.}\right], \tag{3.90}$$

where I have defined a new mode function $\boldsymbol{v}_l(\boldsymbol{r})$ as

$$\boldsymbol{v}_l(\boldsymbol{r})\equiv\sum_j\omega_j^{1/2}W_{jl}\boldsymbol{u}_j(\boldsymbol{r})\propto\sum_{\boldsymbol{k},s}\omega_{\boldsymbol{k}}^{1/2}W_{(\boldsymbol{k},s)l}\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \tag{3.91}$$

which is a **superposition of sinusoidal waves**. Each $\hat{b}_l$ is the annihilation operator of a new optical mode with mode function $\boldsymbol{v}_l(\boldsymbol{r})$. In particular, the average $\langle\psi|\,\hat{b}_l\,|\psi\rangle$ determines the average complex amplitude in front of $\boldsymbol{v}_l(\boldsymbol{r})$ in the average electric field $\langle\psi|\,\hat{\boldsymbol{E}}(\boldsymbol{r},0)\,|\psi\rangle$.

W_{jl} as a function of $j=(\boldsymbol{k},s)$ determines the weight of each sinusoidal wave in the expansion of $\boldsymbol{v}_l(\boldsymbol{r})$ given by Eq. (3.91), which resembles a **Fourier series**. We call W_{jl} **the $(\boldsymbol{k},s)$-space amplitude** of the new mode l.

This method is consistent with how we define modes in classical optics, where we define an optical mode as a superposition of sinusoidal waves.

Because W is unitary, Eq. (3.89) implies

$$\boxed{\left[\hat{b}_l,\hat{b}_m\right]=0,}\qquad\qquad\boxed{\left[\hat{b}_l,\hat{b}_m^\dagger\right]=\delta_{lm},} \tag{3.92}$$

so these operators behave the same way as the standard annihilation/creation operators for harmonic oscillators, and we can also think of the new modes as a set of oscillators. The new feature of these new modes is that they **may not be normal modes any more**. To compute the Heisenberg picture of $\hat{b}_l$, first write each $\hat{b}_l$ in terms of the normal-mode $\{\hat{a}_j\}$ as

$$\hat{b}_l=\sum_j(W^{-1})_{lj}\hat{a}_j=\sum_j W_{jl}^*\hat{a}_j, \tag{3.93}$$

where the last step uses the fact that W is unitary so $W^{-1} = W^\dagger$ and $(W^\dagger)_{lj} = W^*_{jl}$. Then the Heisenberg picture is

$$\hat{b}_l(t) \equiv \hat{U}^\dagger(t)\hat{b}_l\hat{U}(t) = \sum_j W^*_{jl}\hat{U}^\dagger(t)\hat{a}_j\hat{U}(t) = \sum_j W^*_{jl}\hat{a}_j \exp(-i\omega_j t) \tag{3.94}$$

$$= \sum_j W^*_{jl}\left[\sum_m W_{jm}\hat{b}_m\right]\exp(-i\omega_j t) = \boxed{\sum_m V_{lm}(t)\hat{b}_m,} \tag{3.95}$$

$$V_{lm}(t) \equiv \sum_j W^*_{jl}W_{jm}\exp(-i\omega_j t). \tag{3.96}$$

We see that the Heisenberg equations of motion for the new modes are **coupled** (except in special cases), so we should consider the new set of modes as **coupled oscillators**.

Remark 3.3. *Beware that † on a c-number matrix, such as W here, means the **conjugate transpose**, so that*

$$(W^\dagger)_{lj} = W^*_{jl}, \tag{3.97}$$

*where $*$ denotes the **entry-wise conjugate**. On the other hand, † on an abstract operator, such as $\hat{a}$, means the **adjoint**; see Appendix B. We use the same symbol † to denote the two different operations depending on the context, but there should be no ambiguity because here we always put hats on operators and resort to the index notation for matrices when clarity is needed. For example, the adjoint of Eq. (3.89) is given by*

$$\hat{a}_j^\dagger = \left(\sum_l W_{jl}\hat{b}_l\right)^\dagger = \sum_l (W_{jl}\hat{b}_l)^\dagger = \sum_l W^*_{jl}\hat{b}_l^\dagger, \tag{3.98}$$

where we need to take the conjugate of each c-number W_{jl} to pull it out of the adjoint.

Exercise 3.11. Verify Eqs. (3.92), given Eq. (3.89) and the fact that W is a unitary matrix.

Exercise 3.12. Show that

$$\sum_l \hat{b}_l^\dagger\hat{b}_l = \sum_j \hat{a}_j^\dagger\hat{a}_j. \tag{3.99}$$

This equation says that the total photon number is conserved regardless of the mode set.

Exercise 3.13. Rewrite the Hamiltonian in terms of $\{\hat{b}_l\}$ and $\{\hat{b}_l^\dagger\}$. Rederive Eqs. (3.95) and (3.96) from this Hamiltonian.

3.5.1. Example: two polarization modes. For a simple concrete example, let's look at two normal modes with the same $\boldsymbol{k} = k\tilde{\boldsymbol{z}}$, with $s = 1, 2$. These are sinusoidal plane waves propagating in the $\tilde{\boldsymbol{z}}$ direction with two polarizations. Suppose that

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},1} = \tilde{\boldsymbol{x}}, \qquad\qquad \tilde{\boldsymbol{e}}_{\boldsymbol{k},2} = \tilde{\boldsymbol{y}}, \tag{3.100}$$

so the first mode is $\tilde{\boldsymbol{x}}$-polarized, and the second mode is $\tilde{\boldsymbol{y}}$-polarized. Write the annihilation operators for these two modes as $\hat{a}_1$ and $\hat{a}_2$, respectively. We can define an alternative set of polarization modes by assuming

$$W = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = W^\dagger, \qquad \hat{b}_1 = \frac{1}{\sqrt{2}}(\hat{a}_1 + \hat{a}_2), \qquad \hat{b}_2 = \frac{1}{\sqrt{2}}(\hat{a}_1 - \hat{a}_2). \tag{3.101}$$

The mode function for the first new mode with annihilation operator $\hat{b}_1$ becomes

$$\boldsymbol{v}_1(\boldsymbol{r}) \propto \sum_j W_{j1}\boldsymbol{u}_j(\boldsymbol{r}) = W_{11}\boldsymbol{u}_1(\boldsymbol{r}) + W_{21}\boldsymbol{u}_2(\boldsymbol{r}) \tag{3.102}$$

$$\propto \frac{1}{\sqrt{2}}\tilde{\boldsymbol{e}}_{\boldsymbol{k},1}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) + \frac{1}{\sqrt{2}}\tilde{\boldsymbol{e}}_{\boldsymbol{k},2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) = \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{y}})\exp(ik_z z), \tag{3.103}$$

which is also linearly polarized, with a new polarization vector $\frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}}+\tilde{\boldsymbol{y}})$. Similarly,

$$\boldsymbol{v}_1(\boldsymbol{r}) = \sum_j W_{j2}\boldsymbol{u}_j(\boldsymbol{r}) = W_{12}\boldsymbol{u}_1(\boldsymbol{r}) + W_{22}\boldsymbol{u}_2(\boldsymbol{r}) \tag{3.104}$$

$$\propto \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}}-\tilde{\boldsymbol{y}})\exp(ik_z z). \tag{3.105}$$

Thus, we have obtained a new set of linear polarization modes with polarization vectors $\frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}}+\tilde{\boldsymbol{y}})$ and $\frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}}-\tilde{\boldsymbol{y}})$, as illustrated by Fig. 3.1.

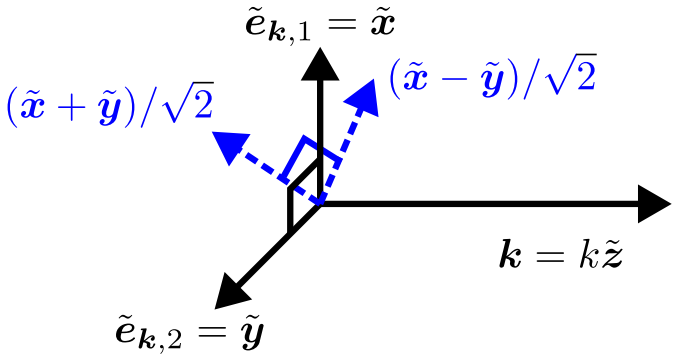

FIGURE 3.1. Given one wavevector $\boldsymbol{k} = k\tilde{\boldsymbol{z}}$ and two polarization modes with polarization vectors $\tilde{\boldsymbol{e}}_{\boldsymbol{k},1} = \tilde{\boldsymbol{x}}$ and $\tilde{\boldsymbol{e}}_{\boldsymbol{k},2} = \tilde{\boldsymbol{y}}$, one can define an alternative set of polarization modes with polarization vectors $(\tilde{\boldsymbol{x}}+\tilde{\boldsymbol{y}})/\sqrt{2}$ and $(\tilde{\boldsymbol{x}}-\tilde{\boldsymbol{y}})/\sqrt{2}$.

This example demonstrates the fundamental fact that there is a lot of freedom in choosing the polarization vectors of the two polarization modes. Using the unitary W matrix, we are free to redefine the polarization modes with polarization vectors that are convenient for a given problem.

Exercise 3.14. If

$$W = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \tag{3.106}$$

what are the new polarizations?

Exercise 3.15. Suppose that two polarization modes have the same $\boldsymbol{k} = k\tilde{\boldsymbol{z}}$ and polarization vectors

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},1} = \tilde{\boldsymbol{x}}, \qquad \tilde{\boldsymbol{e}}_{\boldsymbol{k},2} = \tilde{\boldsymbol{y}}. \tag{3.107}$$

Let their annihilation operators be $\hat{a}_1$ and $\hat{a}_2$, respectively. If we would like to define two new polarization modes with the same $\boldsymbol{k}$ but with polarizations

$$\tilde{\boldsymbol{e}}_{\boldsymbol{k},1} = (\cos\theta)\tilde{\boldsymbol{x}} + (\sin\theta)\tilde{\boldsymbol{y}}, \qquad \tilde{\boldsymbol{e}}_{\boldsymbol{k},2} = (-\sin\theta)\tilde{\boldsymbol{x}} + (\cos\theta)\tilde{\boldsymbol{y}}, \tag{3.108}$$

find the annihilation operators $\hat{b}_1$ and $\hat{b}_2$ for the new modes in terms of $\hat{a}_1$ and $\hat{a}_2$.

Exercise 3.16. If two polarization modes have the same $\boldsymbol{k}$ and two new polarization modes are defined using the formalism in Sec. 3.5.1 with an arbitrary unitary 2×2 matrix W, show that the new modes remain normal modes.

3.5.2. Example: pulse mode. For another example, we focus on the mode function $\boldsymbol{v}_l(\boldsymbol{r})$ for a specific new mode l and choose W_{jl} to be nonzero only for $j = (\boldsymbol{k}, s)$ with $k_x = 0$, $k_y = 0$, and $s = 1$. Then $\boldsymbol{v}_l(\boldsymbol{r})$ is a superposition of sinusoidal waves with the same polarization and all propagating in the $\tilde{\boldsymbol{z}}$ direction, since $\boldsymbol{k} = k_z\tilde{\boldsymbol{z}}$. Assume that $s = 1$ is the polarization with $\tilde{\boldsymbol{e}}_{k_z\tilde{\boldsymbol{z}},1} = \tilde{\boldsymbol{x}}$, and we know that $\omega_j^{1/2} = \sqrt{c|\boldsymbol{k}|} = \sqrt{c|k_z|}$. Then we can write

$$W_{jl} = \delta_{s1}\delta_{k_x 0}\delta_{k_y 0}w_l(k_z), \tag{3.109}$$

where $w_l(k_z)$ is some function of k_z, and the mode function becomes

$$\boldsymbol{v}_l(\boldsymbol{r}) \propto \tilde{\boldsymbol{x}} \sum_{k_z} \sqrt{c|k_z|} w_l(k_z) \exp(ik_z z). \tag{3.110}$$

The sum $\sum_{\boldsymbol{k},s} = \sum_{k_x} \sum_{k_y} \sum_{k_z} \sum_s$ has been simplified to a single sum $\sum_{k_z}$, which is a simple Fourier series, and in the $L \to \infty$ limit it is an **inverse Fourier transform**. For example, suppose that $w_l(k_z)$ looks like

$$w_l(k_z) \propto \operatorname{rect}\left(\frac{k_z - k_0}{\kappa}\right) \exp(-ik_z z_l), \qquad \operatorname{rect} X \equiv \begin{cases} 1, & |X| \le 1/2, \\ 0, & |X| > 1/2, \end{cases} \tag{3.111}$$

where κ, k_0, z_l are all real numbers. In other words, $w_l(k_z)$ is a rectangle with center at $k_z = k_0$ and width equal to κ, multiplied by a phase factor $\exp(-ik_z z_l)$ with a certain constant z_l that depends on the mode index l. If

$$\kappa \ll k_0, \tag{3.112}$$

then $w_l(k_z)$ is a very sharp function centered at $k_z = k_0$, and we may approximate

$$\sqrt{c|k_z|} w_l(k_z) \approx \sqrt{c|k_0|} w_l(k_z). \tag{3.113}$$

By the inverse Fourier transform of a rectangle function, the mode function in real space would look like

$$\boldsymbol{v}_l(\boldsymbol{r}) \propto \tilde{\boldsymbol{x}} \operatorname{sinc}\left[\frac{\kappa}{2\pi}(z - z_l)\right] \exp[ik_0(z - z_l)], \qquad \operatorname{sinc} X \equiv \frac{\sin(\pi X)}{\pi X}. \tag{3.114}$$

This function in real space is localized along z with center at $z = z_l$ and width $\propto 1/\kappa$—a simple model for an **optical pulse**, also called a wavepacket sometimes. See Fig. 3.2 for plots of the rect and sinc functions. The phase factor $\exp[ik_0(z - z_l)]$ models the fact that an optical pulse has rapid oscillations along the z direction under the sinc envelope.

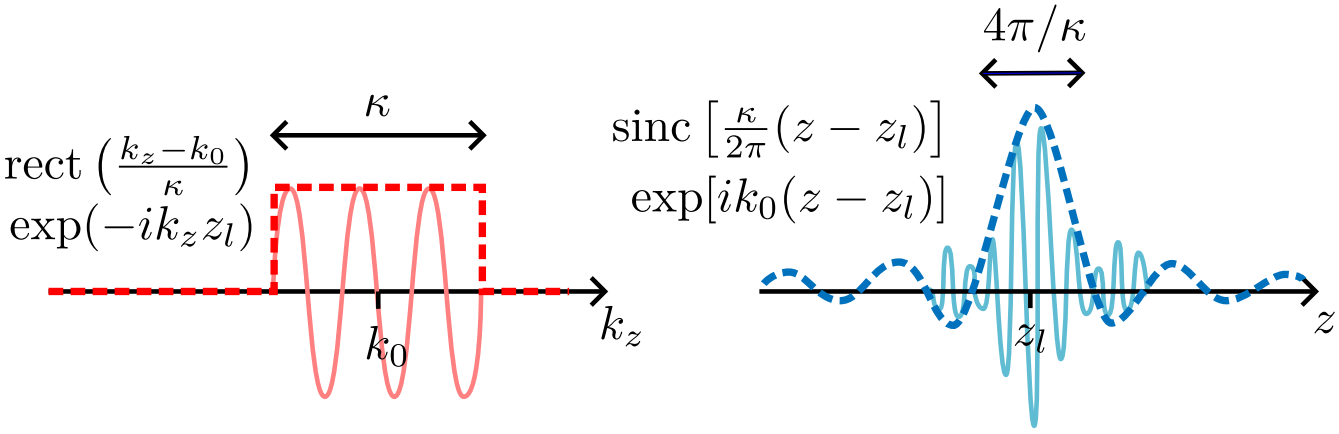

FIGURE 3.2. Functions with rect and sinc envelopes.

In general, we don't have to use the rectangle function for the $(\boldsymbol{k}, s)$-space amplitude. The important point of this example is that the $(\boldsymbol{k}, s)$-space amplitude W_{jl} determines the electric field of a new mode through a Fourier series.

Side note. *Eq. (3.112) comes from the slowly-varying envelope approximation commonly made in optics, when there are many oscillations under the envelope, i.e.,* $\exp(ik_0 z)$ *oscillates rapidly and* $\operatorname{sinc}[\frac{\kappa}{2\pi}(z - z_l)]$ *is relatively slowly varying along* z*.*

Exercise 3.17. Assume the continuum-mode formalism in Sec. 3.4. Define new mode annihilation operators as

$$\boxed{\hat{b}_l = \sum_s \iiint W_l^*(\boldsymbol{k}, s) \hat{a}(\boldsymbol{k}, s) d^3\boldsymbol{k},} \tag{3.115}$$

where each $W_l(\boldsymbol{k}, s)$ is a $(\boldsymbol{k}, s)$-space amplitude of the mode, generalizing W_{jl} in the discrete case.

(1) Find the condition on the functions $\{W_l(\boldsymbol{k}, s)\}$ such that $\{\hat{b}_l\}$ obey the commutation relation given by Eq. (3.92). Prove that

$$\boxed{\sum_s \iiint W_l^*(\boldsymbol{k}, s) W_m(\boldsymbol{k}, s) d^3\boldsymbol{k} = \delta_{lm}.} \tag{3.116}$$

(2) Let

$$W_l(\boldsymbol{k}, s) = \delta_{s1} X(k_x) Y(k_y) Z_l(k_z), \tag{3.117}$$

$$Z_l(k_z) = C \,\mathrm{rect}\left(\frac{k_z - k_0}{\kappa}\right) \exp(-ik_z z_l), \tag{3.118}$$

where $X(k_x)$ and $Y(k_y)$ are some functions that satisfy

$$\int_{-\infty}^{\infty} |X(k_x)|^2 dk_x = 1, \qquad \int_{-\infty}^{\infty} |Y(k_y)|^2 dk_y = 1. \tag{3.119}$$

Find the positive real constant C.

(3) Show that, if

$$z_l = z_0 + \frac{2\pi}{\kappa} l, \tag{3.120}$$

where l is an integer, then Eq. (3.116) is satisfied.

(4) Define

$$\hat{A}(\boldsymbol{r}, s) \equiv \frac{1}{(2\pi)^{3/2}} \iiint \exp(i\boldsymbol{k} \cdot \boldsymbol{r}) \hat{a}(\boldsymbol{k}, s) d^3\boldsymbol{k}. \tag{3.121}$$

(5) Find $\hat{a}(\boldsymbol{k}, s)$ in terms of $\hat{A}(\boldsymbol{r}, s)$.

(6) Find $[\hat{A}(\boldsymbol{r}, s), \hat{A}^\dagger(\boldsymbol{r}', s')]$.

(7) Let

$$\hat{b}_l = \sum_s \iiint \tilde{W}_l^*(\boldsymbol{r}, s) \hat{A}(\boldsymbol{r}, s) d^3\boldsymbol{r}. \tag{3.122}$$

Find the relation between $\tilde{W}_l$ and the W_l in Eq. (3.115). Prove that

$$\sum_s \iiint \tilde{W}_l^*(\boldsymbol{r}, s) \tilde{W}_m(\boldsymbol{r}, s) d^3\boldsymbol{r} = \delta_{lm}. \tag{3.123}$$

(8) Given Eqs. (3.117) and (3.118), find $\tilde{W}_l(\boldsymbol{r}, s)$.

(This exercise gives a precise definition of pulse modes in the continuum formalism, without all the $\approx$ signs and unknown constants. The definition in terms of $\hat{A}(\boldsymbol{r}, s)$ shows that one can just as well define modes using amplitude functions $\{\tilde{W}_l(\boldsymbol{r}, s)\}$ in real space.)

3.5.3. Decomposition of Hilbert space in terms of the new modes. Once we have a new set of modes with annihilation operators $\{\hat{b}_1, \hat{b}_2, \dots\}$, we can define a new orthonormal basis of the Hilbert space. A number state with respect to the new set of modes is defined as

$$|b : n_1, \dots, n_J\rangle \equiv \frac{(\hat{b}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \cdots \frac{(\hat{b}_J^\dagger)^{n_J}}{\sqrt{n_J!}} |\mathrm{vac}\rangle, \quad \text{each } n_l = 0, 1, 2, \dots, \tag{3.124}$$

where $b :$ in the ket emphasizes that it is defined in terms of the $\hat{b}$ operators. Physically, $|b : n_1, \dots, n_J\rangle$ represents a quantum state with n_1 photons in the first new mode, n_2 photons in the second new mode, etc. Exercise 3.18 asks you to prove that this set is also an orthonormal basis of the multimode Hilbert space.

(Note that the orthonormality of the basis relies on the standard commutation relations given by Eqs. (3.92), which follow from our assumption that the W matrix is unitary. This section wouldn't work at all if W weren't unitary!)

We learned earlier in Sec. 3.2 that the multimode Hilbert space $\mathcal{H}$ is constructed from a tensor product of Hilbert spaces $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_J$ of the normal modes. It turns out that we can just as well regard the multimode Hilbert space as a tensor product of Hilbert spaces $\{\mathcal{H}'_l\}$ in terms of the new modes. The mathematical procedure is as follows:

(1) Let $\mathcal{H}'_l$ be a Hilbert space for one new mode labeled by l, with an orthonormal basis denoted as $\{|b_l : n\rangle : n \in \{0, 1, 2, \dots\}\}$. An annihilation operator $\hat{b}$ for this mode is defined in the usual way by

$$\hat{b}\,|b_l : n\rangle = \sqrt{n}\,|b_l : n-1\rangle\,. \tag{3.125}$$

(2) Associate each $|b : n_1, \dots, n_J\rangle$ state in the multimode Hilbert space $\mathcal{H}$ with a product state in $\mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_J$ like this:

$$|b : n_1, \dots, n_J\rangle = |b_1 : n_1\rangle \otimes |b_2 : n_2\rangle \otimes \cdots \otimes |b_J : n_J\rangle\,. \tag{3.126}$$

This association is just like Eq. (3.51): it gives a one-to-one mapping between each $|b : n_1, \dots, n_J\rangle \in \mathcal{H}$ and a product state $|b_1 : n_1\rangle \otimes \cdots \otimes |b_J : n_J\rangle \in \mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_J$. The one-to-one mapping between the two orthonormal bases implies that the two Hilbert spaces are **isomorphic**, and we write

$$\mathcal{H} = \mathcal{H}'_1 \otimes \mathcal{H}'_2 \otimes \cdots \otimes \mathcal{H}'_J. \tag{3.127}$$

(Isomorphic is just a fancy word to say they are the same thing; see Sec. B.9 for a precise definition.)

(3) Since each $\hat{b}_l$ acts on one new mode only and does nothing to all the other modes, i.e.,

$$\hat{b}_l\,|b : \dots, n_l, \dots\rangle = \sqrt{n_l}\,|b : \dots, n_l - 1, \dots\rangle\,, \tag{3.128}$$

we can associate each $\hat{b}_l$ on the multimode Hilbert space $\mathcal{H}$ with a single-mode annihilation operator $\hat{b}$ on $\mathcal{H}'_l$ as follows:

$$\hat{b}_l = \hat{I}'_1 \otimes \cdots \otimes \hat{I}'_{l-1} \otimes \hat{b} \otimes \hat{I}'_{l+1} \otimes \cdots \otimes \hat{I}'_J, \tag{3.129}$$

just like Eq. (3.56), where each $\hat{I}'_l$ is the identity operator on $\mathcal{H}'_l$.

Physically, the modes are the degrees of freedom for EM, and this section says that we are free to choose any set of modes as the degrees of freedom as long as Eq. (3.89) holds with a unitary W as we change from one set to another. We can define a new tensor-product decomposition $\mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_J$ for the multimode Hilbert space, such that the new operators $\{\hat{b}_l\}$ act on the new decomposition $\mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_J$ in the same way as the old operators $\{\hat{a}_j\}$ act on the original decomposition $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_J$. Normal modes are special only because the Hamiltonian in terms of them is simple.

I stress that there is nothing mysterious about changing the degrees of freedom; we do that all the time in classical physics. For example, consider a particle with Cartesian position coordinates $(x, y) \in \mathbb{R}^2$ in 2D. We may change the coordinates to, say, $u = (x + y)/\sqrt{2}$ and $v = (x - y)/\sqrt{2}$, which are Cartesian position coordinates in their own right. A preferred alignment of the coordinate system emerges only if we consider the dynamics, e.g., a force may act on the particle in the $(\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{y}})/\sqrt{2}$ direction, in which case (u, v) are convenient.

For a 2D quantum particle, we have two position operators $\hat{x}$ and $\hat{y}$ on a tensor-product Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, and the change of our Cartesian coordinate system mentioned earlier would lead to new position operators $\hat{u} = (\hat{x} + \hat{y})/\sqrt{2}$ and $\hat{v} = (\hat{x} - \hat{y})/\sqrt{2}$. The physics can't care less how we define our Cartesian coordinate system, so the Hilbert space $\mathcal{H}$ should remain the same, while there should exist a new decomposition of $\mathcal{H}$ as $\mathcal{H}'_1 \otimes \mathcal{H}'_2$ such that $\hat{u}$ and $\hat{v}$ act on them the same way $\hat{x}$ and $\hat{y}$ act on $\mathcal{H}_1 \otimes \mathcal{H}_2$.

The transformation of EM modes follows the same principle; we just have a lot more of them.

Exercise 3.18.

(1) Prove that the set

$$\{|b : n_1, \dots, n_J\rangle : \text{each } n_l = 0, 1, 2, \dots\} \tag{3.130}$$

is orthonormal, i.e., they obey

$$\langle b : m_1, \dots, m_J | b : n_1, \dots, n_J\rangle = \delta_{m_1 n_1}\delta_{m_2 n_2}\dots\delta_{m_J n_J}. \tag{3.131}$$

(2) Prove that Eq. (3.130) is also a basis of the Hilbert space $\mathcal{H}$, meaning that any $|\psi\rangle \in \mathcal{H}$ can be expressed as a linear combination of the set, i.e., for any $|\psi\rangle \in \mathcal{H}$, there exists a wavefunction $\Psi_{n_1\dots n_j}$ such that

$$|\psi\rangle = \sum_{n_1,\dots,n_J} \Psi_{n_1\dots n_j} |b : n_1, \dots, n_J\rangle . \tag{3.132}$$

Exercise 3.19. Suppose that there are just two polarization modes, and follow Sec. 3.5.1. Let

$$|a : n_1, n_2\rangle \equiv \frac{\hat{a}_1^{\dagger n_1}}{\sqrt{n_1!}} \frac{\hat{a}_2^{\dagger n_2}}{\sqrt{n_2!}} |\text{vac}\rangle . \tag{3.133}$$

Assume that W is given by Eq. (3.101).

(1) Write each $|b : n_1, n_2\rangle$ in terms of $\{|a : n_1, n_2\rangle\}$, for total photon number $n_1 + n_2$ up to 2.
(2) Write each $|a : n_1, n_2\rangle$ in terms of $\{|b : n_1, n_2\rangle\}$ for total photon number up to 2.
(3) Repeat (1) and (2) if W is given by Eq. (3.106).

Exercise 3.20. The most general way of defining new modes is to take the new mode annihilation operators $\{\hat{b}_l\}$ to be

$$\hat{b}_l = \hat{U}^\dagger \hat{a}_l \hat{U}, \quad l = 1, \dots, J, \tag{3.134}$$

where $\hat{U}$ is a unitary operator that doesn't depend on l.

(1) Show that the new annihilation operators $\{\hat{b}_l\}$ still obey Eqs. (3.92).
(2) The new vacuum state $|\text{vac}'\rangle$ is defined by

$$\hat{b}_l \left|\text{vac}'\right\rangle = 0 \quad \forall l. \tag{3.135}$$

Find a relation between $|\text{vac}'\rangle$, $\hat{U}$, and the old $|\text{vac}\rangle$.
(3) The new number states are defined by

$$|b : n_1, \dots, n_J\rangle \equiv \frac{\hat{b}_1^{\dagger n_1} \dots \hat{b}_J^{\dagger n_J}}{\sqrt{n_1! \dots n_J!}} \left|\text{vac}'\right\rangle . \tag{3.136}$$

Show that they are an orthonormal basis.
(4) Find a unitary operator $\hat{U}$ such that we retrieve the transformation given by Eq. (3.89) as a special case. (This problem requires Chapter 6.)
(5) The so-called Bogoliubov transformation gives

$$\hat{b}_l = \sum_j \left(C_{lj}\hat{a}_j + S_{lj}\hat{a}_j^\dagger \right). \tag{3.137}$$

Find the conditions on the C and S matrices so that the new annihilation operators still obey Eqs. (3.92).
(6) Find a unitary operator $\hat{U}$ that gives the Bogoliubov transformation.
(7) Find $\hat{a}_j$ in terms of $\{\hat{b}_l\}$ for the Bogoliubov transformation.

CHAPTER 4

Single-Mode States

There are three fundamental ingredients of quantum mechanics/quantum optics:

(1) The initial state modeled by $|\psi\rangle$ or the density operator $\hat{\rho}$ (see Sec. D.6).
(2) The dynamics governed by the Hamiltonian $\hat{H}$.
(3) The measurement.

This chapter and the next will study some common quantum states assumed in quantum optics. To be gentle, this chapter considers only **one EM mode**, which may be a normal mode or a general mode in the sense of Sec. 3.5. We will follow the notation of Sec. 3.1, i.e., the annihilation operator is $\hat{a}$, the creation operator is $\hat{a}^\dagger$, the number operator is $\hat{n} = \hat{a}^\dagger\hat{a}$, the q-quadrature operator is $\hat{q} \equiv (\hat{a} + \hat{a}^\dagger)/\sqrt{2}$, and the p-quadrature operator is $\hat{p} \equiv (\hat{a} - \hat{a}^\dagger)/(\sqrt{2}i)$.

4.1. Number states

The number states $|n\rangle$, $n \in \{0, 1, 2, \dots\}$ have been discussed in Sec. 3.1. The set of all number states $\{|n\rangle : n \in \{0, 1, 2, \dots\}\}$ is an orthonormal basis of the single-mode Hilbert space, i.e., they are orthonormal ($\langle m|n\rangle = \delta_{nm}$) and complete ($\hat{I} = \sum_n |n\rangle\langle n|$). We also know that each $|n\rangle$ is an eigenstate of the photon-number operator $\hat{n} \equiv \hat{a}^\dagger\hat{a}$ with eigenvalue n ($\hat{n}|n\rangle = n|n\rangle$). $|0\rangle$, in particular, is called the vacuum state. We use a letter n or m to denote a number state $|n\rangle$ usually. It is also called a Fock state sometimes.

Recall that $|q = x\rangle$ is an eigenstate of the q-quadrature operator $\hat{q} \equiv (\hat{a} + \hat{a}^\dagger)/\sqrt{2}$ with eigenvalue x. The q-quadrature wavefunction of each number state turns out to be

$$\langle q = x|n\rangle = \frac{1}{\sqrt{2^n n!}\pi^{1/4}} H_n(x) \exp\left(-\frac{x^2}{2}\right), \tag{4.1}$$

which is a Hermite-Gaussian function and H_n is the Hermite polynomial of degree n (https://en.wikipedia.org/wiki/Hermite_polynomials), as is well known from kindergarten quantum mechanics.

The problem with number states is that it is extremely difficult to observe or prepare them in a real experiment and they are just a terrible model of the quantum state of light from any common light source (sun, stars, LEDs, lasers, etc.). For example, if we measure the photon number in an optical mode generated by a common light source, we would always find a random outcome following some probability distribution, e.g., Poisson or exponential. The result of measuring the photon number of a number state $|n\rangle$, on the other hand, will always be deterministic and exactly equal to n.

Another problem is that a number state always gives zero mean fields, so it is difficult to reproduce classical EM with number states. From Exercise 3.3, you should have found that $\langle n|\hat{q}|n\rangle = 0$ and $\langle n|\hat{p}|n\rangle = 0$. These results would mean that $\langle n|\hat{a}|n\rangle = 0$ and $\langle n|\hat{a}^\dagger|n\rangle = 0$, and the average EM fields for the optical mode $\langle n|\hat{\boldsymbol{E}}|n\rangle$ and $\langle n|\hat{\boldsymbol{B}}|n\rangle$ would also be zero.

Exercise 4.1. Assume a number state $|n\rangle$.

(1) Find the probability distribution of the photon number $\hat{n}$.
(2) Find the probability density of $\hat{q}$.
(3) Find the probability density of $\hat{p}$.

(The probability distribution of an observable $\hat{A}$ is defined as the probability distribution of the outcome if a von Neumann measurement of $\hat{A}$ is performed; see Appendix D for a quick review.)

4.2. Coherent states

To make quantum optics agree with classical EM, the simplest quantum state one can assume is a coherent state. It is commonly denoted by $|\alpha\rangle$ with a greek letter α or β, where $\alpha \in \mathbb{C}$ is a complex parameter that determines all the properties of the state. We call α the **amplitude** of the coherent state. In terms of the number states $\{|n\rangle : n = 0, 1, 2, \dots\}$, it is defined as

$$\boxed{|\alpha\rangle \equiv \exp\left(-\frac{|\alpha|^2}{2}\right) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle .} \tag{4.2}$$

An interesting and useful property of a coherent state is that it is an eigenstate of the annihilation operator $\hat{a}$ and the eigenvalue is α:

$$\boxed{\hat{a} |\alpha\rangle = \alpha |\alpha\rangle .} \tag{4.3}$$

Conversely, any eigenstate of $\hat{a}$ is a coherent state with amplitude equal to the eigenvalue. Since $\hat{a}$ is not a Hermitian operator, a von Neumann measurement of $\hat{a}$ is undefined, but we can measure the quadratures, and the expected values of $\hat{q}$ and $\hat{p}$ are given by

$$\boxed{\langle q\rangle \equiv \langle\alpha| \hat{q} |\alpha\rangle = \frac{1}{\sqrt{2}}(\alpha + \alpha^*) = \sqrt{2}\,\mathrm{Re}\,\alpha,} \tag{4.4}$$

$$\boxed{\langle p\rangle \equiv \langle\alpha| \hat{p} |\alpha\rangle = \frac{1}{\sqrt{2}i}(\alpha - \alpha^*) = \sqrt{2}\,\mathrm{Im}\,\alpha.} \tag{4.5}$$

These relations are reminiscent of the relation between the quadratures and the complex amplitude for an optical mode in classical optics, as discussed in Chapter 2, except that here the relations hold for the expected values of $\hat{q}$ and $\hat{p}$. Unlike a number state, we can get any values of $\langle q\rangle$ and $\langle p\rangle$ for a coherent state by choosing its complex paramater α. By assuming a coherent state for each mode ($|\alpha\rangle = \bigotimes_j |\alpha_j\rangle$), we can get back classical EM if we look at the mean fields $\langle\alpha| \hat{\boldsymbol{E}} |\alpha\rangle$ and $\langle\alpha| \hat{\boldsymbol{B}} |\alpha\rangle$.

Side note. *The coherent states were first proposed by Schrödinger, but the importance of coherent states to quantum optics was first recognized by Glauber, who won a Nobel prize for that insight.*

An important feature of quantum mechanics is that a measurement outcome is random usually, so we shouldn't just look at its mean, we should study the probability distribution as well. A nice property of coherent states is that it gives simple probability distributions for common measurements.

(1) The probability distribution of the photon number $\hat{n}$ is given by

$$\boxed{|\langle n|\alpha\rangle|^2 = \exp\bigl(-|\alpha|^2\bigr)\frac{|\alpha|^{2n}}{n!},} \tag{4.6}$$

which is a **Poisson distribution with mean number** $|\alpha|^2$. See the top row of Fig. 4.1 for some plots.

(2) The probability density of the q-quadrature operator $\hat{q}$ is

$$\boxed{|\langle q = x|\alpha\rangle|^2 = \frac{1}{\sqrt{\pi}} \exp\left[-\Bigl(x - \sqrt{2}\,\mathrm{Re}\,\alpha\Bigr)^2\right],} \tag{4.7}$$

which is a **Gaussian probability density with mean** $\sqrt{2}\,\mathrm{Re}\,\alpha$ **and variance** $1/2$ (see Sec. C.6 for a quick review).

(3) Similarly, the probability density of the p-quadrature operator $\hat{p}$ is

$$\boxed{|\langle p = y|\alpha\rangle|^2 = \frac{1}{\sqrt{\pi}} \exp\left[-\Bigl(y - \sqrt{2}\,\mathrm{Im}\,\alpha\Bigr)^2\right].} \tag{4.8}$$

We can no longer think of a quantum coherent state as just a single point in phase space in the classical picture (Fig. 2.3). There are uncertainties in both quadratures if we measure them.

The Poissonian or Gaussian noise modeled by these probability distributions for a coherent state is commonly called the **quantum shot noise**.

Exercise 4.2. Verify that Eq. (4.2) is normalized, i.e., $\langle\alpha|\alpha\rangle = 1$.

Exercise 4.3.

(1) Show that a coherent state $|\alpha\rangle$ with $\alpha = 0$ is identical to the vacuum state $|n\rangle$ with $n = 0$, so no confusion arises if we write $|0\rangle$.
($|q = 0\rangle$ and $|p = 0\rangle$, on the other hand, are different, so we need the notation $q =$ and $p =$ to be clear.)

(2) Find the photon-number distribution $|\langle n|\alpha\rangle|^2$ and show that, as $\alpha \to 0$, it is the same as the photon-number distribution $|\langle n|0\rangle|^2$ for the vacuum state.

Exercise 4.4. Verify Eqs. (4.3)–(4.5).

Exercise 4.5. Derive Eq. (4.2) from Eq. (4.3). This means that Eq. (4.3) can also be used as a definition of a coherent state.

Exercise 4.6. Find the variance of the photon number if the probability distribution is given by Eq. (4.6).

Exercise 4.7. Compute the variances

$$\left\langle \Delta q^2 \right\rangle \equiv \langle\alpha|\,\hat{q}^2\,|\alpha\rangle - (\langle\alpha|\,\hat{q}\,|\alpha\rangle)^2, \qquad \left\langle \Delta p^2 \right\rangle \equiv \langle\alpha|\,\hat{p}^2\,|\alpha\rangle - (\langle\alpha|\,\hat{p}\,|\alpha\rangle)^2 \tag{4.9}$$

directly, without using Eqs. (4.7) and (4.8). Your answers should agree with the variances of the probability densities given by Eqs. (4.7) and (4.8). Show that the variances obey the uncertainty relation

$$\left\langle \Delta q^2 \right\rangle \left\langle \Delta p^2 \right\rangle \geq C, \tag{4.10}$$

where C is a constant you should derive.

Exercise 4.8. Let the fractional variance of an observable be $\left\langle \Delta O^2 \right\rangle / \langle O \rangle^2$. Compute the fractional variance of $\hat{n}$, $\hat{q}$, and $\hat{p}$ for a coherent state $|\alpha\rangle$ and show that it approaches 0 as $\mathrm{Re}\,\alpha \to \infty$ and $\mathrm{Im}\,\alpha \to \infty$, i.e., the observables are increasingly deterministic for large α. (We get back classical EM with no noise in this limit.)

Exercise 4.9. A quantum covariance of two observables $\hat{A}$ and $\hat{B}$ can be defined as

$$\mathrm{COV}(\hat{A}, \hat{B}) \equiv \langle\psi|\,\hat{A} \circ \hat{B}\,|\psi\rangle - \Big(\langle\psi|\,\hat{A}\,|\psi\rangle\Big)\Big(\langle\psi|\,\hat{B}\,|\psi\rangle\Big), \tag{4.11}$$

where $\circ$ is called the Jordan product, defined as

$$\hat{A} \circ \hat{B} \equiv \frac{1}{2}\Big(\hat{A}\hat{B} + \hat{B}\hat{A}\Big). \tag{4.12}$$

Compute $\mathrm{COV}(\hat{q}, \hat{p})$ for a coherent state $|\alpha\rangle$.

Exercise 4.10. Compute the expected value of the photon number

$$\langle n \rangle \equiv \langle\alpha|\,\hat{n}\,|\alpha\rangle \tag{4.13}$$

for a coherent state and the variance, defined as

$$\left\langle \Delta n^2 \right\rangle \equiv \langle\alpha|\,\hat{n}^2\,|\alpha\rangle - (\langle\alpha|\,\hat{n}\,|\alpha\rangle)^2. \tag{4.14}$$

Answer: for the variance, you should obtain

$$\boxed{\left\langle \Delta n^2 \right\rangle = \langle n \rangle\,.} \tag{4.15}$$

Exercise 4.11. Given two coherent states $|\alpha\rangle$ and $|\beta\rangle$, compute $\langle\alpha|\beta\rangle$.

Exercise 4.12. Show

$$\hat{I} = \frac{1}{\pi} \iint |\alpha\rangle \langle\alpha| \, d^2\alpha, \qquad\qquad d^2\alpha \equiv (d \operatorname{Re}\alpha)(d \operatorname{Im}\alpha). \tag{4.16}$$

$d^2\alpha$ means that we treat any function of α as a function of two real variables: $\operatorname{Re}\alpha$ and $\operatorname{Im}\alpha$, and the integration is over the 2D complex plane.

(This identity means that any state can be expressed as a linear combination of coherent states given by

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \frac{1}{\pi} \iint |\alpha\rangle \langle\alpha|\psi\rangle \, d^2\alpha, \tag{4.17}$$

so $\{|\alpha\rangle : \alpha \in \mathbb{C}\}$ is a complete vector set of the Hilbert space, even though the elements are not orthogonal to each other.)

Exercise 4.13. Let the Hamiltonian be the harmonic-oscillator Hamiltonian

$$\hat{H} = \hbar\omega \hat{a}^\dagger \hat{a}. \tag{4.18}$$

If the initial state is a coherent state $|\alpha\rangle$, find the state in the Schrödinger picture after time t, i.e., compute

$$\exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\alpha\rangle\,. \tag{4.19}$$

4.3. Displacement operator

There's a lovely way of writing the coherent state in terms of the so-called displacement operator $\hat{D}(\alpha)$ and the vacuum state $|0\rangle$:

$$\boxed{|\alpha\rangle = \hat{D}(\alpha)\,|0\rangle\,,} \tag{4.20}$$

$$\boxed{\hat{D}(\alpha) \equiv \exp\left(\alpha\hat{a}^\dagger - \alpha^*\hat{a}\right).} \tag{4.21}$$

The displacement operator is very useful in itself. You should convince yourself that $\hat{D}(\alpha)$ is unitary, and

$$\hat{D}^\dagger(\alpha) = \hat{D}(-\alpha). \tag{4.22}$$

It is called a displacement operator mainly because of what it does to $\hat{a}$ in the Heisenberg picture:

$$\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha) = \hat{a} + \alpha. \tag{4.23}$$

Then it's easy to show

$$\hat{D}^\dagger(\alpha)\hat{q}\hat{D}(\alpha) = \hat{q} + \sqrt{2}\operatorname{Re}\alpha, \tag{4.24}$$

$$\hat{D}^\dagger(\alpha)\hat{p}\hat{D}(\alpha) = \hat{p} + \sqrt{2}\operatorname{Im}\alpha. \tag{4.25}$$

In other words, the displacement operator is a special unitary that displaces the quadrature operators in the Heisenberg picture by c-numbers, depending on the α parameter. Another useful property is

$$\boxed{\hat{D}(\alpha)\hat{D}(\beta) = e^{i\operatorname{Im}(\beta^*\alpha)}\hat{D}(\alpha+\beta).} \tag{4.26}$$

The exponential factor $e^{i\operatorname{Im}(\beta^*\alpha)}$ is an unimportant c-number phase factor that won't show up in the Heisenberg picture, i.e.,

$$\hat{D}^\dagger(\alpha)\hat{D}^\dagger(\beta)\hat{A}\hat{D}(\beta)\hat{D}(\alpha) = \hat{D}^\dagger(\alpha+\beta)\hat{A}\hat{D}(\alpha+\beta), \tag{4.27}$$

so the total effect of two displacements is the same as the effect of one net displacement.

We will see throughout this book that the displacement operator is very handy when doing math concerning a coherent state.

Exercise 4.14. Show that $\hat{D}(\alpha)$ is unitary. Verify Eq. (4.22).

Exercise 4.15. Use the Baker-Campbell-Hausdorff (BCH) formula (https://en.wikipedia.org/wiki/Baker%E2%80%93Campbell%E2%80%93Hausdorff_formula) to show

$$\hat{D}(\alpha) = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} = e^{\frac{1}{2}|\alpha|^2} e^{-\alpha^* \hat{a}} e^{\alpha \hat{a}^\dagger}. \tag{4.28}$$

Exercise 4.16. Verify Eqs. (4.20), (4.23)–(4.25).

Exercise 4.17. A displacement operator can also be expressed as

$$\exp(i\xi\hat{q} - i\eta\hat{p}), \tag{4.29}$$

where ξ and η are real numbers.

(1) If we want to write this as $\hat{D}(\alpha)$, find ξ and η in terms of α.

(2) Using the BCH formula, one can write

$$\exp(i\xi\hat{q} - i\eta\hat{p}) = c\exp(i\xi\hat{q})\exp(-i\eta\hat{p}) = d\exp(-i\eta\hat{p})\exp(i\xi\hat{q}). \tag{4.30}$$

where c and d are complex numbers. Find c and d.

(3) Find

$$\hat{D}(\alpha)\left|q = x\right\rangle, \quad \hat{D}(\alpha)\left|p = y\right\rangle. \tag{4.31}$$

(4) Verify Eqs. (4.6)–(4.8).

Exercise 4.18. Let

$$\hat{q}' \equiv \hat{D}^\dagger(\alpha)\hat{q}\hat{D}(\alpha) \tag{4.32}$$

be the Heisenberg picture of q-quadrature operator $\hat{q}$ after displacement. Show that the variance of $\hat{q}'$ remains the same, i.e.,

$$\left\langle \Delta q'^2 \right\rangle \equiv \langle\psi| (\hat{q}')^2 |\psi\rangle - \left(\langle\psi|\hat{q}'|\psi\rangle\right)^2 \tag{4.33}$$

is the same as $\left\langle \Delta q^2 \right\rangle$ for any state $|\psi\rangle$.

4.4. Thermal states

We need to use a density operator $\hat{\rho}$ (see Sec. D.6) to describe the thermal state. Quantum thermodynamics tells us that, when a system is in thermal equilibrium with some bath and only energy is exchanged with the bath, the quantum state of the system (excluding the bath) is given by the Gibbs state

$$\hat{\rho} = \frac{1}{Z}\exp\left(-\beta\hat{H}\right), \qquad \beta \equiv \frac{1}{k_B T}, \qquad Z \equiv \mathrm{tr}\left[\exp\left(-\beta\hat{H}\right)\right], \tag{4.34}$$

where $\hat{H}$ is the Hamiltonian of the system, k_B is Boltzmann constant, T is the temperature, tr is the operator trace (see Appendix B for the definition), and Z is called the partition function if we regard it as a function of β. For example, if we have a resonator and we leave it alone at some temperature, then the EM modes in the resonator should be in the thermal state. We may think of Z as just a constant to normalize the density operator ($\mathrm{tr}\,\hat{\rho} = 1$). For one normal mode with natural frequency ω, $\hat{H} = \hbar\omega\hat{n}$, so $\hat{\rho}$ can be expressed as

$$\boxed{\hat{\rho} = \frac{1}{Z}\exp(-\beta\hbar\omega\hat{n}),} \qquad \boxed{Z = \mathrm{tr}\left[\exp(-\beta\hbar\omega\hat{n})\right].} \tag{4.35}$$

Recall that we can write the number operator $\hat{n}$ in the diagonal form (Appendix B)

$$\hat{n} = \sum_{n=0}^{\infty} n\left|n\right\rangle\left\langle n\right|. \tag{4.36}$$

Any function of $\hat{n}$ is then defined as

$$f(\hat{n}) = \sum_{n=0}^{\infty} f(n)\left|n\right\rangle\left\langle n\right|, \tag{4.37}$$

and the trace of such a function becomes

$$\mathrm{tr}[f(\hat{n})] = \sum_{n=0}^{\infty} f(n). \tag{4.38}$$

It follows that another way of writing $\hat{\rho}$ for a thermal state is

$$\hat{\rho} = \sum_{n=0}^{\infty} \frac{1}{Z} \exp(-\beta\hbar\omega n) \left|n\right\rangle \left\langle n\right| = \sum_{n=0}^{\infty} P_n \left|n\right\rangle \left\langle n\right|. \tag{4.39}$$

We can think of this $\hat{\rho}$ as a mixture of photon-number states, and the mixing probability distribution P_n is the exponential distribution

$$P_n = \frac{1}{Z} \exp(-\beta\hbar\omega n). \tag{4.40}$$

With the thermal state, the probability distribution of $\hat{n}$ coincides with P_n:

$$\left\langle n\right| \hat{\rho} \left|n\right\rangle = P_n. \tag{4.41}$$

In particular, the mean photon number is

$$\langle n\rangle \equiv \mathrm{tr}\left(\hat{n}\hat{\rho}\right) = \sum_{n=0}^{\infty} n \left\langle n\right| \hat{\rho} \left|n\right\rangle = \sum_{n=0}^{\infty} nP_n = \boxed{\frac{1}{\exp(\beta\hbar\omega) - 1}}, \tag{4.42}$$

which agrees with **Bose-Einstein** statistics. In terms of $\langle n\rangle$, $\hat{\rho}$ and P_n can also be expressed as

$$\hat{\rho} = \frac{1}{\langle n\rangle + 1} \left(\frac{\langle n\rangle}{\langle n\rangle + 1}\right)^{\hat{n}}, \qquad\qquad P_n = \frac{1}{\langle n\rangle + 1} \left(\frac{\langle n\rangle}{\langle n\rangle + 1}\right)^{n}. \tag{4.43}$$

See the bottom row of Fig. 4.1 for some plots.

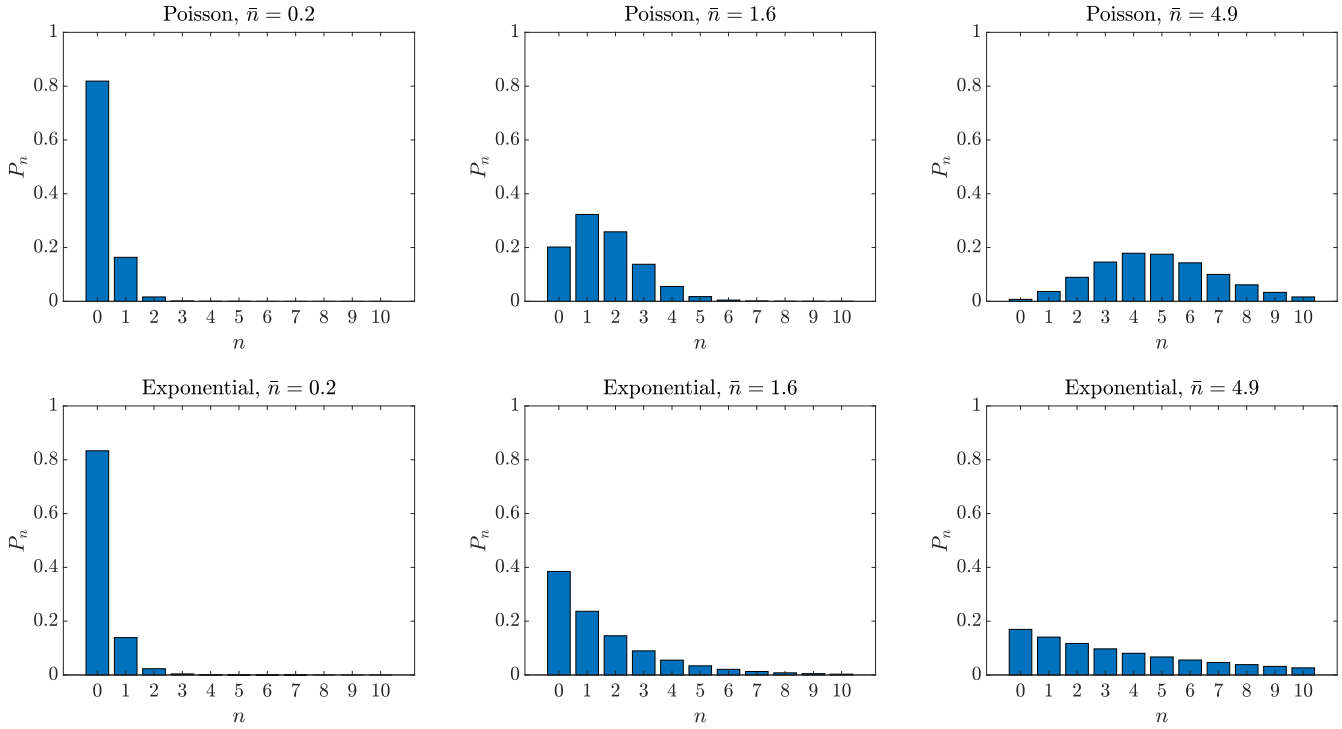

FIGURE 4.1. Plots of the Poisson distribution for coherent states (top row) and the exponential distribution for thermal states (bottom row) for some mean photon numbers $\langle n\rangle$.

A fundamental result discovered by Glauber is that the thermal state can also be expressed as a **mixture of coherent states**:

$$\textbf{Glauber's formula:} \quad \boxed{\hat{\rho} = \iint \Phi(\alpha) \left|\alpha\right\rangle \left\langle\alpha\right| d^2\alpha,} \qquad d^2\alpha \equiv (d\,\mathrm{Re}\,\alpha)(d\,\mathrm{Im}\,\alpha), \tag{4.44}$$

where the mixing probability density is a Gaussian given by

$$\boxed{\Phi(\alpha) = \frac{1}{\pi \left\langle n\right\rangle} \exp\left(-\frac{|\alpha|^2}{\left\langle n\right\rangle}\right),} \tag{4.45}$$

so we can also think of a thermal state as a **noisy coherent state**, where the complex amplitude α is a **zero-mean complex Gaussian random variable**.

One nice thing about Glauber's formula is that the quadrature probability densities

$$\left\langle q = x\right| \hat{\rho} \left|q = x\right\rangle, \quad \left\langle p = y\right| \hat{\rho} \left|p = y\right\rangle \tag{4.46}$$

become simple to compute for a thermal state.

Exercise 4.19. Convince yourself that

$$Z = \sum_{m=0}^{\infty} \exp(-\beta\hbar\omega m) = \frac{1}{1 - \exp(-\beta\hbar\omega)} = \left\langle n\right\rangle + 1. \tag{4.47}$$

Exercise 4.20.

(1) Find the photon-number distribution P_n for a thermal state as $\beta\hbar\omega \to \infty$ (infinite ω or zero temperature).
(2) Show that, as $\beta\hbar\omega \to \infty$, the thermal state approaches the vacuum state, viz.,

$$\boxed{\lim_{\beta\hbar\omega\to\infty} \hat{\rho} \to \left|0\right\rangle \left\langle 0\right|.} \tag{4.48}$$

Exercise 4.21. Find the variance of the photon number for a thermal state in terms of $\left\langle n\right\rangle$. The variance is defined as

$$\left\langle \Delta n^2 \right\rangle \equiv \mathrm{tr}\left(\hat{n}^2\hat{\rho}\right) - \left[\mathrm{tr}\left(\hat{n}\hat{\rho}\right)\right]^2. \tag{4.49}$$

Answer: you should obtain

$$\boxed{\left\langle \Delta n^2 \right\rangle = \left\langle n\right\rangle + \left\langle n\right\rangle^2.} \tag{4.50}$$

This is larger than the variance of the coherent state given by Eq. (4.15), meaning that a thermal state is "noisier" than a coherent state with the same mean photon number $\left\langle n\right\rangle$. When $\left\langle n\right\rangle \ll 1$, however, this variance is close to the Poissonian variance $\left\langle n\right\rangle$.

Exercise 4.22. Let $T = 300$ K (room temperature). Find the mean photon number $\left\langle n\right\rangle$ and the probability $P[n \geq 1]$ that the photon number is nonzero for a thermal state if

(1) $\nu = 2.4$ GHz (microwave frequency)
(2) Free-space wavelength $\lambda = 1,550$ nm (typical wavelength for optical fiber communication).

Conversely, if we desire $\left\langle n\right\rangle = 0.01$, find the temperature T for each case above.

(The low average photon number and low $P[n \geq 1]$ at optical frequencies at typical temperatures is the main reason why we can usually assume a vacuum initial state in quantum optics.)

Exercise 4.23. Compute the probability that the measured photon number is equal to 2 for a coherent state with mean photon number $\left\langle n\right\rangle$. Do the same for a thermal state with the same mean photon number. Expand each result in Taylor series for $\left\langle n\right\rangle \ll 1$ and show that the probability of measuring two photons in a thermal state is approximately **twice** the probability of measuring two photons in a coherent state. This effect is called **bunching**.

Side note. *In the 1950s, people were really confused that weak thermal light doesn't show Poissonian photon-counting statistics exactly and the probability of counting two photons in one mode is higher than expected. The bunching effect was explained first by Leonard Mandel [5] using semiclassical optics, and then Glauber estalished the quantum formalism to explain bunching [6].*

Exercise 4.24. Verify that $\iint \Phi(\alpha) d^2\alpha = 1$, so that Φ is really a probability density function.

Exercise 4.25. Compute the probability densities given by Eqs. (4.46) for a thermal state. Use them to find the means and variances of the quadratures:

$$\langle q \rangle \equiv \mathrm{tr}\,(\hat{q}\hat{\rho}), \qquad \langle p \rangle \equiv \mathrm{tr}\,(\hat{p}\hat{\rho}), \tag{4.51}$$

$$\left\langle \Delta q^2 \right\rangle \equiv \mathrm{tr}\left(\hat{q}^2\hat{\rho}\right) - [\mathrm{tr}(\hat{q}\hat{\rho})]^2, \qquad \left\langle \Delta p^2 \right\rangle \equiv \mathrm{tr}\left(\hat{p}^2\hat{\rho}\right) - [\mathrm{tr}(\hat{p}\hat{\rho})]^2. \tag{4.52}$$

Exercise 4.26. Define a unitary operator as

$$\hat{R}(\theta) \equiv \exp(-i\hat{n}\theta), \tag{4.53}$$

where θ is a real number.

(1) Find

$$\hat{a}(\theta) \equiv \hat{R}^\dagger(\theta)\hat{a}\hat{R}(\theta), \qquad \hat{q}(\theta) \equiv \hat{R}^\dagger(\theta)\hat{q}\hat{R}(\theta), \qquad \hat{p}(\theta) \equiv \hat{R}^\dagger(\theta)\hat{p}\hat{R}(\theta) \tag{4.54}$$

in terms of $\hat{a}$ and θ. $\hat{q}(\theta)$ and $\hat{p}(\theta)$ are also called quadrature operators.

(2) Show that

$$|q(\theta) = x\rangle \equiv \hat{R}^\dagger(\theta)\,|q = x\rangle \tag{4.55}$$

is an eigenstate of $\hat{q}(\theta)$ with eigenvalue x, and

$$|p(\theta) = y\rangle \equiv \hat{R}^\dagger(\theta)\,|p = y\rangle \tag{4.56}$$

is an eigenstate of $\hat{p}(\theta)$ with eigenvalue y.

(3) Show

$$\langle q(\theta) = x | q(\theta) = x' \rangle = \delta(x - x'), \qquad \langle p(\theta) = y | p(\theta) = y' \rangle = \delta(y - y'), \tag{4.57}$$

and the completeness conditions

$$\hat{I} = \int_{-\infty}^{\infty} |q(\theta) = x\rangle \langle q(\theta) = x|\, dx, \qquad \hat{I} = \int_{-\infty}^{\infty} |p(\theta) = y\rangle \langle p(\theta) = y|\, dy. \tag{4.58}$$

In other words, $\{|q(\theta) = x\rangle : x \in \mathbb{R}\}$ is an orthonormal basis (in the sense of Dirac), and so is $\{|p(\theta) = y\rangle : y \in \mathbb{R}\}$.

(4) Show that $\hat{q}(\theta)$ and $\hat{p}(\theta)$ have the diagonal forms

$$\hat{q}(\theta) = \int_{-\infty}^{\infty} x\,|q(\theta) = x\rangle \langle q(\theta) = x|\, dx, \tag{4.59}$$

$$\hat{p}(\theta) = \int_{-\infty}^{\infty} y\,|p(\theta) = y\rangle \langle p(\theta) = y|\, dy. \tag{4.60}$$

(Once we have the diagonal forms, we know that the outcome of a von Neumann measurement of $\hat{q}(\theta)$ would have probability density $\langle q(\theta) = x|\,\hat{\rho}\,|q(\theta) = x\rangle$, and the outcome of a von Neumann measurement of $\hat{p}(\theta)$ would have probability density $\langle p(\theta) = y|\,\hat{\rho}\,|p(\theta) = y\rangle$.)

(5) Compute

$$\hat{R}(\theta)\,|\alpha\rangle\,. \tag{4.61}$$

Your answer should be a coherent state with another complex amplitude.

(6) Find the probability density of $\hat{q}(\theta)$ given a coherent state $|\alpha\rangle$, i.e., compute

$$|\langle q(\theta) = x|\alpha\rangle|^2. \tag{4.62}$$

Do the same for $\hat{p}(\theta)$.

(The point of this exercise is to show that any quadrature of a coherent state has a Gaussian distribution with variance $1/2$.)

(7) Find the probability density of $\hat{q}(\theta)$ given a thermal state. Do the same for $\hat{p}(\theta)$.

4.5. Sudarshan representation

In quantum optics, there exist many different definitions of whether a state is considered classical or nonclassical. Since a coherent state gives results very close to classical EM (Gaussian statistics for quadratures, Poisson statistics for photon number), it is considered a classical state by any definition. If a quantum state is given by a mixture of coherent states, i.e.,

$$\hat{\rho} = \iint \Phi(\alpha)\, |\alpha\rangle\, \langle\alpha|\, d^2\alpha, \tag{4.63}$$

where $\Phi(\alpha)$ is a probability density (i.e., nonnegative for all α), then it is also commonly considered as a classical state, since it's just a noisy coherent state with a random amplitude α, and quantum calculations often agree with classical optics.

Sudarshan discovered that, in general, given any $\hat{\rho}$, it is always possible to derive a formula for $\Phi(\alpha)$, so any state can be written in the form of Eq. (4.63) in principle. $\Phi(\alpha)$ is hence called the **Sudarshan representation** of the quantum state (also called the Glauber-Sudarshan representation or the P function sometimes).

The important caveat is that, for certain quantum states, $\Phi(\alpha)$ may go **negative and very weird** (consisting of derivatives of the Dirac delta function; see https://en.wikipedia.org/wiki/Glauber-Sudarshan_P_representation), so we can no longer regard Eq. (4.63) as a mixture of coherent states, and classical optics no longer works as well. For this reason, a state is often called **nonclassical whenever $\Phi(\alpha)$ goes negative for some value of α**.

Side note. *In this book, we always use P to denote a probability distribution. Since the Sudarshan representation may go negative, we use the symbol Φ rather than P.*

For most common light sources, such as lasers, LEDs, lamps, stars, fluorescent particles, Eq. (4.63) with a nonnegative Φ works very well, the noise due to Φ is often much stronger than the quantum shot noise, and there is no good reason to use the quantum theory. An important exception is when photon counting that is close to ideal can be performed. The probability distribution of the photon count becomes

Mandel's formula :
$$\boxed{\langle n|\,\hat{\rho}\,|n\rangle = \iint \Phi(\alpha)|\langle n|\alpha\rangle|^2 d^2\alpha = \iint \Phi(\alpha)\exp\left(-|\alpha|^2\right)\frac{|\alpha|^{2n}}{n!}d^2\alpha.} \tag{4.64}$$

The measurement outcome must remain discrete, with $n = 0, 1, 2, \ldots$. If Φ is nonnegative, Eq. (4.64) is called a **semiclassical** formula, since we can regard the complex amplitude α as a classical random variable with probability density $\Phi(\alpha)$ and the Poissonian $|\langle n|\alpha\rangle|^2$ as the probability distribution of the photon number conditioned on α. In other words, if Φ is nonnegative, we can treat the EM fields as classical and stochastic, and the discreteness of photon number appears only when a photon-number measurement is performed.

Exercise 4.27. Show that $\Phi(\alpha)$ must obey

$$\iint \Phi(\alpha) d^2\alpha = 1, \tag{4.65}$$

regardless of whether it's a probability density.

Exercise 4.28. Let $\langle n\rangle \equiv \mathrm{tr}(\hat{n}\hat{\rho})$ be the mean photon number. Given Eq. (4.63) where Φ is a probability density, show that the photon-number variance given by Eq. (4.49) must obey

$$\left\langle \Delta n^2 \right\rangle \geq \langle n\rangle \,. \tag{4.66}$$

In other words, the variance cannot go below the variance of a Poisson random variable. If the variance goes below $\langle n\rangle$, then it's a smoking gun that Φ for the state cannot be a probability density. Use this fact to show that Φ for a number state $\hat{\rho} = |n\rangle\langle n|$ with $n > 0$ cannot be a probability density.

Hint: use the law of total variance (see https://en.wikipedia.org/wiki/Law_of_total_variance or Eq. (C.48)).

4.6. Normal ordering and optical equivalence theorem

Suppose that we are given an operator in the form

$$f(\hat{a}^\dagger)g(\hat{a}), \tag{4.67}$$

where $f(\hat{a}^\dagger)$ is a function of $\hat{a}^\dagger$ only and $g(\hat{a})$ is a function of $\hat{a}$ only. We call this a **normally ordered operator**, with all the $\hat{a}^\dagger$ on the left and all the $\hat{a}$ on the right. Some examples:

$$\hat{a}^\dagger\hat{a}, \quad \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}, \quad \exp\left(u\hat{a}^\dagger\right)\exp(v^*\hat{a}). \tag{4.68}$$

Then it can be shown that

$$\boxed{\mathrm{tr}\left[f(\hat{a}^\dagger)g(\hat{a})\hat{\rho}\right] = \iint \Phi(\alpha)f(\alpha^*)g(\alpha)d^2\alpha,} \tag{4.69}$$

where we replace $\hat{a}^\dagger$ in $f(\hat{a}^\dagger)$ by the variable α^* and $\hat{a}$ in $g(\hat{a})$ by α on the right-hand side. In other words, the expected value of a normally-ordered operator can be computed by taking the average of the c-number function $f(\alpha^*)g(\alpha)$ using the Sudarshan Φ. Eq. (4.69) is called the optical equivalence theorem, which is a handy result in quantum optics.

Exercise 4.29.

(1) Verify Eq. (4.69).
(2) Let
$$\hat{A} = \hat{n}^2 = \hat{a}^\dagger\hat{a}\hat{a}^\dagger a. \tag{4.70}$$
Rewrite it in normal-ordering form (i.e., a sum of terms in the form of Eq. (4.67)) and compute $\langle A\rangle \equiv \mathrm{tr}(\hat{A}\hat{\rho})$ using the optical equivalence theorem for a coherent state and a thermal state.
(3) Compute $\langle A\rangle$ directly using the photon-number distributions of a coherent state (Poisson) and a thermal state. Confirm that you obtain the same results as the previous part.

Exercise 4.30.

(1) Show that the Poisson distribution can be expanded as a power series with respect to $\langle n\rangle$ given by
$$\exp(-\langle n\rangle)\frac{\langle n\rangle^n}{n!} = \frac{1}{n!}\Big(\langle n\rangle^n - \langle n\rangle^{n+1} + \dots\Big). \tag{4.71}$$
(2) Show
$$\langle n=1|\,\hat{\rho}\,|n=1\rangle = \mathrm{tr}\left(\hat{a}^\dagger\hat{a}\hat{\rho}\right) - \mathrm{tr}\left(\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\hat{\rho}\right) + \dots \tag{4.72}$$
$$\langle n=2|\,\hat{\rho}\,|n=2\rangle = \frac{1}{2}\Big[\mathrm{tr}\left(\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\hat{\rho}\right) - \mathrm{tr}\left(\hat{a}^\dagger\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\hat{a}\hat{\rho}\right) + \dots\Big]. \tag{4.73}$$
(This is a way of computing $\langle n=1|\,\hat{\rho}\,|n=1\rangle$ and $\langle n=2|\,\hat{\rho}\,|n=2\rangle$ for weak light in any state, generalizing Exercise 4.23.)

CHAPTER 5

Multimode States

EM fields have many modes, and the real fun starts in quantum optics when we consider many modes. This chapter studies some common multimode states in quantum optics, generalizing Chapter 4.

5.1. Coherent states

5.1.1. Definition in terms of the displacement operator. Let's consider J EM modes and denote each mode by $j = 1, 2, \ldots, J$. The annihilation operator for mode j is $\hat{a}_j$, as before. The easiest way to define a coherent state for multiple modes is to first define a multimode displacement operator as

$$\boxed{\hat{D}(\boldsymbol{\alpha}) \equiv \exp\left[\sum_j \left(\alpha_j \hat{a}_j^\dagger - \text{H.c.}\right)\right],} \tag{5.1}$$

where

$$\boldsymbol{\alpha} \equiv \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_J \end{pmatrix} \in \mathbb{C}^J \tag{5.2}$$

is a vectoral complex amplitude (each α_j is a complex number) and H.c. denotes the Hermitian conjugate of the first term $\alpha_j \hat{a}_j^\dagger$, i.e., $\alpha_j^* \hat{a}_j$ in this case. Because operators for different modes commute with one another (see Eqs. (3.59)), the BCH formula says we can break $\hat{D}(\boldsymbol{\alpha})$ into a product of single-mode displacement operators

$$\hat{D}(\boldsymbol{\alpha}) = \hat{D}_1(\alpha_1) \ldots \hat{D}_J(\alpha_J), \tag{5.3}$$

$$\hat{D}_j(\alpha_j) \equiv \exp\Big(\alpha_j \hat{a}_j^\dagger - \text{H.c.}\Big). \tag{5.4}$$

Each $\hat{D}_j(\alpha_j)$ is in terms of $\hat{a}_j$ and $\hat{a}_j^\dagger$ only, so it acts only on mode j and does nothing on all other modes.

A multimode coherent state can now be defined as

$$\boxed{|\boldsymbol{\alpha}\rangle = \hat{D}(\boldsymbol{\alpha}) |\text{vac}\rangle,} \tag{5.5}$$

where $|\text{vac}\rangle$ is the multimode vacuum state (zero photon in all modes). The coherent state has some special properties.

5.1.2. Separability. Let the Hilbert space for mode j be $\mathcal{H}_j$ and each number state in $\mathcal{H}_j$ be $|n_j\rangle_j$, $n_j = 0, 1, 2, \ldots$. Recall that the vacuum state is a tensor product of $\{|0\rangle_j\}$:

$$|\text{vac}\rangle = |0\rangle_1 \otimes |0\rangle_2 \otimes \cdots \otimes |0\rangle_J. \tag{5.6}$$

We see from Eq. (5.4) that each $\hat{D}_j(\alpha_j)$ acts on $\mathcal{H}_j$ only and has no effect on all the other modes. So $\hat{D}(\boldsymbol{\alpha}) |\text{vac}\rangle$ becomes

$$|\boldsymbol{\alpha}\rangle = \hat{D}(\alpha_1) |0\rangle_1 \otimes \hat{D}(\alpha_2) |0\rangle_2 \otimes \cdots \otimes \hat{D}(\alpha_J) |0\rangle_J \tag{5.7}$$

$$= \boxed{|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_J\rangle.} \tag{5.8}$$

In other words, a multimode coherent state is a **tensor product of single-mode coherent states**.

This separable property of the coherent state turns out to hold regardless of the set of modes we assume. Recall from Sec. 3.5 that we can build our multimode Hilbert space using any set of modes, as long as the new operators are related to the old operators by

$$\hat{a}_j = \sum_l W_{jl}\hat{b}_l, \qquad \hat{b}_l = \sum_j W^*_{jl}\hat{a}_j, \tag{5.9}$$

where W is a unitary matrix ($W^{-1} = W^\dagger$). Let's plug this expression into Eq. (5.1) to obtain

$$\hat{D}(\boldsymbol{\alpha}) = \exp\left[\sum_l \left(\beta_l \hat{b}_l^\dagger - \text{H.c.}\right)\right], \tag{5.10}$$

$$\beta_l \equiv \sum_j \alpha_j W^*_{jl}. \tag{5.11}$$

Notice that the displacement operator has the same dependence on $\{\hat{b}_l\}$ as it did on $\{\hat{a}_j\}$, except that the amplitudes $\{\beta_j\}$ are transformed. To make the notation clearer, let's write

$$\hat{D}(a:\boldsymbol{\alpha}) \equiv \exp\left[\sum_j \left(\alpha_j \hat{a}_j^\dagger - \text{H.c.}\right)\right], \qquad \hat{D}(b:\boldsymbol{\beta}) \equiv \exp\left[\sum_l \left(\beta_l \hat{b}_l^\dagger - \text{H.c.}\right)\right], \qquad \boldsymbol{\beta} \equiv \begin{pmatrix}\beta_1 \\ \vdots \\ \beta_J\end{pmatrix}, \tag{5.12}$$

to clarify the dependence of a displacement operator on the mode operators. In matrix notation, Eq. (5.11) can be expressed as

$$\boldsymbol{\beta} = W^\dagger \boldsymbol{\alpha}, \tag{5.13}$$

so that Eq. (5.10) becomes

$$\boxed{\hat{D}(a:\boldsymbol{\alpha}) = \hat{D}(b:W^\dagger\boldsymbol{\alpha}),} \tag{5.14}$$

and the coherent state can now be expressed as

$$\boxed{|\boldsymbol{\alpha}\rangle \equiv \hat{D}(a:\boldsymbol{\alpha})\,|\text{vac}\rangle = \hat{D}(b:W^\dagger\boldsymbol{\alpha})\,|\text{vac}\rangle\,.} \tag{5.15}$$

We now follow Sec. 5.1.2 to write the multimode Hilbert space as $\mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_J$ for the new modes. Write the vacuum state in terms of the zero-number states in $\mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_J$ as

$$|\text{vac}\rangle = |b_1:0\rangle \otimes |b_2:0\rangle \otimes \cdots \otimes |b_J:0\rangle \tag{5.16}$$

according to Eqs. (3.124) and (3.126). Then decompose $\hat{D}(b:\boldsymbol{\beta})$ as

$$\hat{D}(b:\boldsymbol{\beta}) = \hat{D}(b_1:\beta_1)\ldots\hat{D}(b_J:\beta_J), \qquad \hat{D}(b_l,\beta_l) \equiv \exp\left(\beta_l \hat{b}_l^\dagger - \text{H.c.}\right), \tag{5.17}$$

just like Eq. (5.3). The coherent state becomes

$$\hat{D}(b:\boldsymbol{\beta})\,|\text{vac}\rangle = \hat{D}(b_1:\beta_1)\ldots\hat{D}(b_J:\beta_J)\,|b_1:0\rangle \otimes \cdots \otimes |b_J:0\rangle \tag{5.18}$$

$$= \hat{D}(b_1:\beta_1)\,|b_1:0\rangle \otimes \cdots \otimes \hat{D}(b_J:\beta_J)\,|b_J:0\rangle \tag{5.19}$$

$$= |b_1:\beta_1\rangle \otimes \cdots \otimes |b_J:\beta_J\rangle\,, \quad |b_j:\beta_j\rangle \equiv \hat{D}(b:\beta_j)\,|b_j:0\rangle\,, \tag{5.20}$$

which is a tensor product of coherent states. This separable property is very special, since it says that the multimode coherent state remains **pure and a coherent state** if we look at any set of modes, normal or not, or any subset of the modes.

5.1.3. Single-mode excitation. Given a vectoral complex amplitude $\boldsymbol{\alpha}$, suppose that we define a special set of modes such that the first new mode has an annihilation operator given by

$$\hat{b}_1 = \sum_j W_{j1}^* \hat{a}_j = \frac{1}{|\boldsymbol{\alpha}|} \sum_j \alpha_j^* \hat{a}_j, \tag{5.21}$$

$$W_{j1} = \frac{\alpha_j}{|\boldsymbol{\alpha}|}, \tag{5.22}$$

where the norm of the vectoral amplitude $\boldsymbol{\alpha}$ is defined by

$$|\boldsymbol{\alpha}|^2 \equiv \boldsymbol{\alpha}^\dagger \boldsymbol{\alpha} = \sum_j |\alpha_j|^2. \tag{5.23}$$

In other words, we choose a unitary matrix W such that its first column is equal to $\boldsymbol{\alpha}/|\boldsymbol{\alpha}|$. The normalization $1/|\boldsymbol{\alpha}|$ ensures that W can remain unitary and $\hat{b}_1$ obeys the standard commutation relation $[\hat{b}_1, \hat{b}_1^\dagger] = 1$. (It can be shown using linear algebra that it's always possible to fill the remaining columns of W to make it unitary.) Then the displacement operator can be rewritten as

$$\hat{D}(\boldsymbol{\alpha}) = \exp\left[|\boldsymbol{\alpha}|\left(\hat{b}_1^\dagger - \hat{b}_1\right)\right], \tag{5.24}$$

which is in terms of $\hat{b}_1$ only. In other words, in terms of this new special set of modes, $\hat{D}(\boldsymbol{\alpha})$ displaces only the first mode, while leaving all the other modes alone. For this reason, the coherent state

$$|\boldsymbol{\alpha}\rangle = \hat{D}(\boldsymbol{\alpha})\,|\text{vac}\rangle = \exp\left[|\boldsymbol{\alpha}|\left(\hat{b}_1^\dagger - \hat{b}_1\right)\right]|\text{vac}\rangle \tag{5.25}$$

can also be considered as **a state with excitation in one special mode only**, while all the other modes remain in vacuum. We call this special mode the **excited mode** of the coherent state.

If $\{\hat{a}_j\}$ are operators for normal sinusoidal-wave modes in free space, recall from Sec. 3.5 that W_{j1} is the $(\boldsymbol{k}, s)$-space amplitude that determines the mode function $\boldsymbol{v}_1(\boldsymbol{r})$ for the excited mode. This means that the excited mode has a $(\boldsymbol{k}, s)$-space amplitude W_{j1} determined by $\boldsymbol{\alpha}$ through Eq. (5.22). For example, if $\boldsymbol{\alpha}$ is the $(\boldsymbol{k}, s)$-space amplitude of an optical pulse, as discussed in Sec. 3.5, then $W_{j1} \propto \alpha_j$ is also the $(\boldsymbol{k}, s)$-space amplitude of an optical pulse, and the excited mode is the optical pulse mode.

Exercise 5.1. Prove the following:

(1)

$$\boxed{\hat{a}_j\,|\boldsymbol{\alpha}\rangle = \alpha_j\,|\boldsymbol{\alpha}\rangle\,.} \tag{5.26}$$

(2)

$$\boxed{\langle\boldsymbol{\alpha}|\,\hat{a}_j^\dagger = \alpha_j^*\,\langle\boldsymbol{\alpha}|\,.} \tag{5.27}$$

(3)

$$\boxed{\hat{D}(\boldsymbol{\alpha}) = \hat{D}^\dagger(-\boldsymbol{\alpha}).} \tag{5.28}$$

(4)

$$\boxed{\hat{D}(\boldsymbol{\alpha})\hat{D}(\boldsymbol{\beta}) = \exp\left[i\,\text{Im}(\boldsymbol{\beta}^\dagger\boldsymbol{\alpha})\right]\hat{D}(\boldsymbol{\alpha}+\boldsymbol{\beta}),} \tag{5.29}$$

(5)

$$\boxed{\langle\boldsymbol{\alpha}|\boldsymbol{\beta}\rangle = \exp\left[-i\,\text{Im}(\boldsymbol{\beta}^\dagger\boldsymbol{\alpha})\right]\exp\left(-\frac{1}{2}|\boldsymbol{\beta}-\boldsymbol{\alpha}|^2\right).} \tag{5.30}$$

(6)

$$\boxed{\hat{D}(\boldsymbol{\alpha}) = e^{-\frac{1}{2}|\boldsymbol{\alpha}|^2} e^{\sum_j \alpha_j \hat{a}_j^\dagger} e^{-\sum_j \alpha_j^* \hat{a}_j} = e^{\frac{1}{2}|\boldsymbol{\alpha}|^2} e^{-\sum_j \alpha_j^* \hat{a}_j} e^{\sum_j \alpha_j \hat{a}_j^\dagger}.} \tag{5.31}$$

Exercise 5.2. Find the probability distribution of multimode photon counting for a coherent state, i.e.,

$$|\langle \boldsymbol{n}|\boldsymbol{\alpha}\rangle|^2, \tag{5.32}$$

where

$$\boldsymbol{n} \equiv \begin{pmatrix} n_1 \\ \vdots \\ n_J \end{pmatrix}, \qquad\qquad |\boldsymbol{n}\rangle \equiv |n_1, \ldots, n_J\rangle\,. \tag{5.33}$$

Define the multimode quadrature eignstates as

$$|q = \boldsymbol{x}\rangle \equiv |q_1 = x_1\rangle \otimes \cdots \otimes |q_J = x_J\rangle\,, \qquad |p = \boldsymbol{y}\rangle \equiv |p_1 = y_1\rangle \otimes \cdots \otimes |p_J = y_J\rangle\,. \tag{5.34}$$

where $|q_j = x_j\rangle$ is an eigenstate of $\hat{q}_j$ with eigenvalue x_j and $|p_j = x_j\rangle$ is an eigenstate of $\hat{p}_j$ with eigenvalue y_j in the usual way. Find the probability density functions

$$|\langle q = \boldsymbol{x}|\boldsymbol{\alpha}\rangle|^2, \quad |\langle p = \boldsymbol{y}|\boldsymbol{\alpha}\rangle|^2. \tag{5.35}$$

5.2. Classical current source

We love the coherent state in quantum optics—its math is simple, and it's easy to reproduce classical optics by taking its averages. This section presents another reason: it has a very simple model for how it can be generated.

Suppose that, in addition to the free EM fields, there exists a current density $\boldsymbol{J}(\boldsymbol{r}, t)$ due to charged particles that can be approximated as a **c-number function**. The approximation of observables as c-numbers is common in quantum mechanics and valid whenever some degrees of freedom are little perturbed by any coupling to quantum systems and can be approximated as classical. The Hamiltonian can be taken as

$$\hat{H}(t) = \hat{H}_{\text{easy}} + \hat{\eta}(t), \qquad \hat{H}_{\text{easy}} = \sum_j \hbar\omega_j \hat{a}_j^\dagger \hat{a}_j, \qquad \boxed{\hat{\eta}(t) = -\iiint \boldsymbol{J}(\boldsymbol{r}, t) \cdot \hat{\boldsymbol{A}}(\boldsymbol{r}) d^3\boldsymbol{r},} \tag{5.36}$$

where

$$\hat{\boldsymbol{A}}(\boldsymbol{r}) = \sum_j \left(\frac{\hbar}{2\epsilon_0\omega_j}\right)^{1/2} [\hat{a}_j \boldsymbol{u}_j(\boldsymbol{r}) + \text{H.c.}] \tag{5.37}$$

is the vector-potential operator. Appendix E explains the origin of Eq. (5.37) and shows that the Hamiltonian is consistent with Maxwell's equations in the presence of the current density. Going to the interaction picture (see Sec. D.4), we find

$$\hat{\eta}_{\text{easy}}(\tau) = -\iiint \boldsymbol{J}(\boldsymbol{r}, t) \cdot \hat{\boldsymbol{A}}(\boldsymbol{r}, t) d^3\boldsymbol{r}, \tag{5.38}$$

$$\hat{U}_I(t) \equiv \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^t \hat{\eta}_{\text{easy}}(\tau) d\tau\right] = \mathcal{T} \exp\left\{\sum_j \int_0^t \Big[\beta_j(\tau)\hat{a}_j^\dagger - \text{H.c.}\Big] d\tau\right\}, \tag{5.39}$$

$$\beta_j(\tau) \equiv i\left(\frac{1}{2\hbar\omega_j\epsilon_0}\right)^{1/2} \iiint \boldsymbol{J}(\boldsymbol{r}, \tau) \cdot \boldsymbol{u}_j^*(\boldsymbol{r}) \exp(i\omega_j\tau) d^3\boldsymbol{r}. \tag{5.40}$$

The time-ordered exponential looks scary, but remember that it is simply a product of exponentials with tiny time steps:

$$\begin{aligned}\hat{U}_I(t) = \lim_{\Delta t \to 0} &\exp\left\{\sum_j \Big[\beta_j(t)\hat{a}_j^\dagger - \text{H.c.}\Big]\Delta t\right\} \exp\left\{\sum_j \Big[\beta_j(t - \Delta t)\hat{a}_j^\dagger - \text{H.c.}\Big]\Delta t\right\} \ldots \\ &\exp\left\{\sum_j \Big[\beta_j(2\Delta t)\hat{a}_j^\dagger - \text{H.c.}\Big]\Delta t\right\} \exp\left\{\sum_j \Big[\beta_j(\Delta t)\hat{a}_j^\dagger - \text{H.c.}\Big]\Delta t\right\}.\end{aligned} \tag{5.41}$$

Each exponential here is a displacement operator. Recall from Eq. (5.29) that the product of displacement operators is just one displacement operator (with an unimportant phase factor), so $\hat{U}_I(t)$ is in fact a displacement operator, and the EM state resulting from $\hat{U}_I(t)$ applied to an initial EM vacuum state $|\text{vac}\rangle$ is a coherent state. According to Eq. (5.29), the net displacement is the sum of all the tiny displacements, i.e.,

$$\hat{U}_I(t) \propto \hat{D}(\boldsymbol{\alpha}), \tag{5.42}$$

$$\alpha_j = \sum_m \beta_j(m\Delta t)\Delta t \to \int_0^t \beta_j(\tau)d\tau \tag{5.43}$$

$$= i\left(\frac{1}{2\hbar\omega_j\epsilon_0}\right)^{1/2} \int_0^t \iiint \boldsymbol{J}(\boldsymbol{r},\tau)\cdot\boldsymbol{u}_j^*(\boldsymbol{r})\exp(i\omega_j\tau)d^3\boldsymbol{r}d\tau \tag{5.44}$$

$$= i\left(\frac{1}{2\hbar\omega_j\epsilon_0 L^3}\right)^{1/2} \int_0^t \iiint \boldsymbol{J}(\boldsymbol{r},\tau)\cdot\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}^*\exp(-i\boldsymbol{k}\cdot\boldsymbol{r}+i\omega_j\tau)d^3\boldsymbol{r}d\tau. \tag{5.45}$$

This 4D integral can be regarded as an inner product of the current density with a mode function $\boldsymbol{u}_j(\boldsymbol{r})\exp(-i\omega_j\tau)$ with mode index $j=(\boldsymbol{k},s)$. The integral also resembles an inverse Fourier transform of the current density, if we take the limit $t\to\infty$ and $L\to\infty$. The resulting amplitude α_j is the amplitude of the sinusoidal-wave mode $j=(\boldsymbol{k},s)$ generated by the current source.

Long story short, the Hamiltonian $\hat{\eta}_{\text{easy}}(t)$ in the interaction picture is a linear function of $\{\hat{a}_j\}$ and $\{\hat{a}_j^\dagger\}$, so the interaction-picture unitary $\hat{U}_I(t)$ is a displacement operator, and the interaction-picture state $\hat{U}_I(t)\,|\text{vac}\rangle$ is a coherent state. If we wish, we can turn the interaction-picture state back to the Schrödinger picture by applying $\hat{U}_{\text{easy}}(t)$, since

$$\hat{U}(t)\,|\text{vac}\rangle = \hat{U}_{\text{easy}}(t)\hat{U}_{\text{easy}}^\dagger(t)\hat{U}(t)\,|\text{vac}\rangle = \hat{U}_{\text{easy}}(t)\hat{U}_I(t)\,|\text{vac}\rangle\,, \tag{5.46}$$

but it is straightforward to show that $\hat{U}_{\text{easy}}(t)$ applied to a coherent state is still a coherent state.

5.3. Thermal states

5.3.1. Definition. The quantum state at thermal equilibrium with a bath is given by Eq. (4.34) in general, i.e., $\hat{\rho}$ is an exponential of the Hamiltonian $\hat{H}$. Recall that the Hamiltonian for many EM modes in free space is given by Eq. (3.61). It follows that $\hat{\rho}$ can be expressed as

$$\boxed{\hat{\rho} = \frac{1}{Z}\exp\left(-\beta\sum_j \hbar\omega_j\hat{n}_j\right),} \tag{5.47}$$

where $\hat{n}_j$ is the photon-number operator for the normal mode labeled by j. Assume, for simplicity, that there are J normal modes. The number operators all commute with one another ($[\hat{n}_j,\hat{n}_l]=0$), so we can break the exponential into a product of exponentials:

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hbar\omega_1\hat{n}_1)\exp(-\beta\hbar\omega_2\hat{n}_2)\ldots\exp(-\beta\hbar\omega_J\hat{n}_J). \tag{5.48}$$

It can be shown using linear algebra that the density operator can be expressed as the **tensor product**

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hbar\omega_1\hat{n})\otimes\exp(-\beta\hbar\omega_2\hat{n})\otimes\cdots\otimes\exp(-\beta\hbar\omega_J\hat{n}), \tag{5.49}$$

where each $\hat{n}$ is now the number operator on the individual $\mathcal{H}_j$ for each mode. In other words, the normal modes in a thermal state are **independent**. Another way of writing this expression is

$$\boxed{\hat{\rho} = \frac{1}{Z}\left(\frac{\langle n_1\rangle}{\langle n_1\rangle + 1}\right)^{\hat{n}_1} \cdots \left(\frac{\langle n_J\rangle}{\langle n_J\rangle + 1}\right)^{\hat{n}_J},} \tag{5.50}$$

$$Z = \prod_{j=1}^{J}(\langle n_j\rangle + 1), \tag{5.51}$$

where the average photon number in each mode can be expressed as

$$\operatorname{tr}(\hat{n}_j\hat{\rho}) = \langle n_j\rangle = \frac{1}{\exp(\beta\hbar\omega_j) - 1}, \tag{5.52}$$

just as before.

Glauber's formula for a thermal state in J modes is now

Glauber's formula: $$\boxed{\hat{\rho} = \int \Phi(\boldsymbol{\alpha}) \left|\boldsymbol{\alpha}\right\rangle \left\langle\boldsymbol{\alpha}\right| d^{2J}\boldsymbol{\alpha},} \qquad d^{2J}\boldsymbol{\alpha} \equiv \prod_{j=1}^{J}(d\operatorname{Re}\alpha_j)(d\operatorname{Im}\alpha_j), \tag{5.53}$$

where the Φ distribution is given by

$$\boxed{\Phi(\boldsymbol{\alpha}) = \prod_{j=1}^{J}\frac{1}{\pi\langle n_j\rangle}\exp\left(-\frac{|\alpha_j|^2}{\langle n_j\rangle}\right).} \tag{5.54}$$

Φ now coincides with the Gaussian probability density for J independent Gaussian complex random variables.

Exercise 5.3. Verify Eq. (5.51) from the fact that $\operatorname{tr}\hat{\rho} = 1$.

Exercise 5.4. Consider only modes with the same natural frequency $\omega_j = \omega$. Define a new set of modes by Eq. (3.89), where W is a unitary matrix.

(1) Prove

$$\sum_j \hat{a}_j^\dagger\hat{a}_j = \sum_l \hat{b}_l^\dagger\hat{b}_l. \tag{5.55}$$

(2) Let $\hat{m}_l \equiv \hat{b}_l^\dagger\hat{b}_l$. Show that the density operator of the thermal state can be expressed as

$$\hat{\rho} = \frac{1}{Z}\left(\frac{\langle n\rangle}{\langle n\rangle + 1}\right)^{\hat{m}_1} \cdots \left(\frac{\langle n\rangle}{\langle n\rangle + 1}\right)^{\hat{m}_J}, \tag{5.56}$$

so any set of modes with the same frqeuency in the thermal state are independent.

Exercise 5.5. Repeat Exercise 5.2 for a thermal state, i.e., find

$$\left\langle\boldsymbol{n}\right|\hat{\rho}\left|\boldsymbol{n}\right\rangle, \quad \left\langle q = \boldsymbol{x}\right|\hat{\rho}\left|q = \boldsymbol{x}\right\rangle, \quad \left\langle p = \boldsymbol{y}\right|\hat{\rho}\left|p = \boldsymbol{y}\right\rangle \tag{5.57}$$

for a thermal state $\hat{\rho}$.

5.4. Sudarshan representation

Our earlier discussion of the Sudarshan representation applies essentially unchanged to the case of multiple modes. For any density operator $\hat{\rho}$, we can in principle write

$$\boxed{\hat{\rho} = \int \Phi(\boldsymbol{\alpha}) \left|\boldsymbol{\alpha}\right\rangle \left\langle\boldsymbol{\alpha}\right| d^{2J}\boldsymbol{\alpha}.} \tag{5.58}$$

If $\Phi(\boldsymbol{\alpha})$ is nonnegative for all $\boldsymbol{\alpha} \in \mathbb{C}^{2J}$ such that it is a probability density, the state can be called classical.

Mandel's formula in this case is

$$\textbf{Mandel's formula}: \quad \boxed{\langle \boldsymbol{n}| \hat{\rho} |\boldsymbol{n}\rangle = \int \Phi(\boldsymbol{\alpha}) |\langle \boldsymbol{n}|\boldsymbol{\alpha}\rangle|^2 d^{2J}\boldsymbol{\alpha},} \tag{5.59}$$

where

$$\boxed{|\langle \boldsymbol{n}|\boldsymbol{\alpha}\rangle|^2 = \prod_{j=1}^{J} \exp\bigl(-|\alpha_j|^2\bigr) \frac{|\alpha_j|^{2n_j}}{n_j!}} \tag{5.60}$$

is a product of Poisson distributions. If Φ is nonnegative, we can think of the complex amplitudes $\boldsymbol{\alpha}$ as classical random variables with probability density Φ in Mandel's formula, and the photon-number distribution $|\langle \boldsymbol{n}|\boldsymbol{\alpha}\rangle|^2$ conditioned on $\boldsymbol{\alpha}$ is that of independent Poisson random variables.

Exercise 5.6. Show that

$$\int \Phi(\boldsymbol{\alpha}) d^{2J}\boldsymbol{\alpha} = 1. \tag{5.61}$$

5.5. Optical equivalence theorem

The concept of normal ordering and optical equivalence theorem for multiple modes is essentially the same as that discussed in Sec. 4.6. Suppose that we have a **normally ordered operator**

$$f(\hat{a}^\dagger) g(\hat{a}), \tag{5.62}$$

where $f(\hat{a}^\dagger)$ is a function of $\{\hat{a}_j^\dagger\}$ only and $g(\hat{a})$ is a function of $\{\hat{a}_j\}$ only. Some examples:

$$\hat{a}_j^\dagger \hat{a}_l, \quad \hat{a}_j^\dagger \hat{a}_l^\dagger \hat{a}_j \hat{a}_l, \quad \exp\left(\sum_j u_j a_j^\dagger\right) \exp\left(\sum_j v_j^* a_j\right). \tag{5.63}$$

Then the optical equivalence theorem is

$$\boxed{\mathrm{tr}\left[f(\hat{a}^\dagger) g(\hat{a}) \hat{\rho}\right] = \int \Phi(\boldsymbol{\alpha}) f(\boldsymbol{\alpha}^*) g(\boldsymbol{\alpha}) d^{2J}\boldsymbol{\alpha},} \tag{5.64}$$

where we replace each $\hat{a}_j^\dagger$ by α_j^* in the f function and each $\hat{a}_j$ by α_j in the g function on the right-hand side. The theorem allows us to evaluate the expected value of a normally ordered operator by taking the average of a c-number with respect to the Φ function.

5.6. Fock representation

5.6.1. Discrete set of modes. When there are a discrete set of modes, a general state can be constructed from the orthonormal number basis given by Eq. (3.51). If we assume a continuum of modes as per Sec. 3.4, on the other hand, it's trickier to construct the Hilbert space. The way forward is to use Fock's method.

To introduce the method, we begin by considering a discrete set of J modes first, and we label the modes by $j = 1, \ldots, J$. We will be building our Hilbert space from the so-called **Fock states**, defined as

$$\boxed{|\text{Fock} : j_1, \ldots, j_N\rangle \equiv \frac{1}{\sqrt{N!}} \hat{a}_{j_N}^\dagger \ldots \hat{a}_{j_1}^\dagger |\text{vac}\rangle\,.} \tag{5.65}$$

In other words, we construct this state by adding one photon to mode j_1 via $\hat{a}_{j_1}^\dagger$, and then adding another photon to mode j_2 via $\hat{a}_{j_2}^\dagger$, etc. There are N photons in total in this state, and

$$\boldsymbol{j} \equiv (j_1, \ldots, j_N) \tag{5.66}$$

is a vector of mode labels for the N photons, with each $j_n \in \{1, \ldots, J\}$. In mathematics, $\boldsymbol{j}$ is called a multi-index (https://en.wikipedia.org/wiki/Multi-index_notation). There are J^N possible values for the multi-index $\boldsymbol{j}$:

$$\boldsymbol{j} \in \{1, \ldots, J\}^N. \tag{5.67}$$

A lot of the Fock states are equal to each other, since the creation operators in Eq. (5.65) all commute with one another and we can interchange their order. The Fock state must therefore remain the same if we exchange any two arguments, i.e.,

$$|\text{Fock} : \ldots, \underbrace{j}_{n\text{th photon}}, \ldots, \underbrace{j'}_{m\text{th photon}} \ldots\rangle = |\text{Fock} : \ldots, \underbrace{j'}_{n\text{th photon}}, \ldots, \underbrace{j}_{m\text{th photon}} \ldots\rangle. \tag{5.68}$$

To study the Fock states, we can write each in terms of a number state $|n_1, \ldots, n_J\rangle$, since both can be written as some creation operators applied to $|\text{vac}\rangle$. Given the mode labels $(j_1, \ldots, j_N)$ for the N photons, let us count the number of photons in a certain mode l and call it $n_l(j_1, \ldots, j_N)$. This is done by counting the number of j_n's that are equal to the given mode index l. An explicit formula is

$$n_l(j_1, \ldots, j_N) \equiv \delta_{j_1 l} + \delta_{j_2 l} + \cdots + \delta_{j_N l}. \tag{5.69}$$

Then, recalling that a number state is given by

$$|n_1, \ldots, n_J\rangle = \frac{\hat{a}_1^{\dagger n_1} \ldots \hat{a}_J^{\dagger n_J}}{\sqrt{n_1! \ldots n_J!}} |\text{vac}\rangle, \tag{5.70}$$

we can rewrite Eq. (5.65) as

$$|\text{Fock} : j_1, \ldots, j_N\rangle = \left[\frac{n_1(\boldsymbol{j})! \ldots n_J(\boldsymbol{j})!}{N!}\right]^{1/2} |n_1(\boldsymbol{j}), \ldots, n_J(\boldsymbol{j})\rangle, \tag{5.71}$$

which can be abbreviated as

$$\boxed{|\text{Fock} : \boldsymbol{j}\rangle = \binom{N}{\boldsymbol{n}(\boldsymbol{j})}^{-1/2} |\boldsymbol{n}(\boldsymbol{j})\rangle,} \tag{5.72}$$

where

$$\binom{N}{\boldsymbol{n}} \equiv \frac{N!}{n_1! \ldots n_J!} \tag{5.73}$$

is the multinomial coefficient.

Side note. *In the literature, any state with a definite photon number in each mode is also called a Fock state, so $|\boldsymbol{n}\rangle$ would also be called a Fock state. To be precise in this section, however, I call only $|\text{Fock} : \boldsymbol{j}\rangle$ a Fock state and I call $|\boldsymbol{n}\rangle$ a number state.*

Using Eq. (5.72), we find that the inner product between two Fock states is given by

$$\langle \text{Fock} : \boldsymbol{j} | \text{Fock} : \boldsymbol{j}' \rangle = \binom{N}{\boldsymbol{n}(\boldsymbol{j})}^{-1} \delta_{\boldsymbol{n}(\boldsymbol{j}), \boldsymbol{n}(\boldsymbol{j}')}. \tag{5.74}$$

This means that the Fock states are not exactly an orthonormal basis and a lot of the Fock states are actually the same, as long as they lead to the same set of photon numbers $\boldsymbol{n}(\boldsymbol{j})$. Conversely, for a given set of photon numbers $\boldsymbol{n}$, there are $\binom{N}{\boldsymbol{n}}$ Fock states that are all equal to one another (https://www.statisticshowto.com/multinomial-coefficient/).

To express any state in terms of the Fock states, let's first consider the projection operator

$$\sum_{\boldsymbol{j} \in \{1, \ldots, J\}^N} |\text{Fock} : \boldsymbol{j}\rangle \langle \text{Fock} : \boldsymbol{j}| = \sum_{\boldsymbol{j} \in \{1, \ldots, J\}^N} \binom{N}{\boldsymbol{n}(\boldsymbol{j})}^{-1} |\boldsymbol{n}(\boldsymbol{j})\rangle \langle \boldsymbol{n}(\boldsymbol{j})|. \tag{5.75}$$

We can divide the set $\{1,\dots,J\}^N$ into subsets, where each subset of mode labels $\boldsymbol{j}$ for the N photons lead to the same set of photon numbers $\boldsymbol{n}(\boldsymbol{j}) = \boldsymbol{m}$:

$$\{\boldsymbol{j} : \boldsymbol{n}(\boldsymbol{j}) = \boldsymbol{m}\} = \{(j_1,\dots,j_N) : n_j(j_1,\dots,j_N) = m_j \text{ for all } j\}. \tag{5.76}$$

Then

$$\sum_{\boldsymbol{j}\in\{1,\dots,J\}^N} |\text{Fock} : \boldsymbol{j}\rangle \langle\text{Fock} : \boldsymbol{j}| = \sum_{\boldsymbol{j}\in\{1,\dots,J\}^N} \binom{N}{\boldsymbol{n}(\boldsymbol{j})}^{-1} |\boldsymbol{n}(\boldsymbol{j})\rangle \langle\boldsymbol{n}(\boldsymbol{j})| \tag{5.77}$$

$$= \sum_{\boldsymbol{m}:\sum_j m_j = N} \sum_{\boldsymbol{j}:\boldsymbol{n}(\boldsymbol{j})=\boldsymbol{m}} \binom{N}{\boldsymbol{n}(\boldsymbol{j})}^{-1} |\boldsymbol{n}(\boldsymbol{j})\rangle \langle\boldsymbol{n}(\boldsymbol{j})| \tag{5.78}$$

$$= \sum_{\boldsymbol{m}:\sum_j m_j = N} |\boldsymbol{m}\rangle \langle\boldsymbol{m}| . \tag{5.79}$$

We know that the number states $\{|\boldsymbol{n}\rangle\}$ form an orthonormal basis and thus obey the completeness condition

$$\hat{I} = \sum_{\boldsymbol{n}} |\boldsymbol{n}\rangle \langle\boldsymbol{n}| = \sum_{N=0}^{\infty} \sum_{\boldsymbol{n}:\sum n_j = N} |\boldsymbol{n}\rangle \langle\boldsymbol{n}| . \tag{5.80}$$

Hence

$$\boxed{\hat{I} = \sum_{N=0}^{\infty} \sum_{\boldsymbol{j}\in\{1,\dots,J\}^N} |\text{Fock} : \boldsymbol{j}\rangle \langle\text{Fock} : \boldsymbol{j}| .} \tag{5.81}$$

This is a completeness condition in terms of the Fock states, so that an arbitrary $|\psi\rangle \in \mathcal{H}$ can be expressed as

$$|\psi\rangle = \hat{I}|\psi\rangle = \sum_{N=0}^{\infty} \sum_{\boldsymbol{j}\in\{1,\dots,J\}^N} |\text{Fock} : \boldsymbol{j}\rangle \langle\text{Fock} : \boldsymbol{j}|\psi\rangle , \tag{5.82}$$

which is a linear combination of the Fock states. Note, however, that we can't just have any linear combination of $\{|\text{Fock} : \boldsymbol{j}\rangle\}$; the wavefunction $\langle\text{Fock} : \boldsymbol{j}|\psi\rangle$ for N photons must be symmetric with respect to any exchange of two arguments because of Eq. (5.68):

$$\boxed{\langle\text{Fock} : \dots, \underbrace{j}_{n\text{th photon}}, \dots, \underbrace{j'}_{m\text{th photon}} \dots|\psi\rangle = \langle\text{Fock} : \dots, \underbrace{j'}_{n\text{th photon}}, \dots, \underbrace{j}_{m\text{th photon}} \dots|\psi\rangle .} \tag{5.83}$$

This symmetry for the wavefunctions means that the particles are **bosons**, and we have managed to show that a set of quantum oscillators are equivalent to bosons. In the particle picture, each mode label j is associated with the properties of a boson. When the label is $j = (\boldsymbol{k}, s)$, $\boldsymbol{k}$ is regarded as the **momentum** of a boson, and s is regarded as the **spin** of a boson; two possible polarizations of an EM wave correspond to two possible spins for a photon.

A few other formalities: the operators defined as

$$\hat{\Pi}_N \equiv \sum_{\boldsymbol{n}:\sum_j n_j = N} |\boldsymbol{n}\rangle \langle\boldsymbol{n}| = \sum_{\boldsymbol{j}\in\{1,\dots,J\}^N} |\text{Fock} : \boldsymbol{j}\rangle \langle\text{Fock} : \boldsymbol{j}| \tag{5.84}$$

are projection operators that satisfy

$$\hat{\Pi}_N \hat{\Pi}_M = \begin{cases} \hat{\Pi}_N, & N = M, \\ 0, & N \neq M, \end{cases} \qquad \hat{I} = \sum_{N=0}^{\infty} \hat{\Pi}_N. \tag{5.85}$$

The total photon number operator can be expressed as

$$\hat{N} \equiv \sum_j \hat{n}_j = \sum_N N \hat{\Pi}_N, \tag{5.86}$$

and

$$P_N = \mathrm{tr}\left(\hat{\Pi}_N \hat{\rho}\right) \tag{5.87}$$

is the probability that there are N photons in all modes. A normalized N-photon wavefunction can be defined as

$$\psi_N(\boldsymbol{j}) \equiv \frac{1}{\sqrt{P_N}} \langle \text{Fock} : \boldsymbol{j} | \psi \rangle = \frac{1}{\sqrt{P_N N!}} \langle \text{vac} | \, \hat{a}_{j_1} \dots \hat{a}_{j_N} | \psi \rangle \,, \tag{5.88}$$

and

$$|\psi_N(\boldsymbol{j})|^2 = |\psi_N(j_1, \dots, j_N)|^2 \tag{5.89}$$

can be regarded as the probability distribution of random variables $(j_1, \dots, j_N)$, where j_1 is the mode index for the first photon, j_2 is the mode index for the second photon, etc. The probability distribution also needs to stay the same under any exchange of the arguments; we say that the random variables are **exchangeable** in probability theory when the probability distribution has this permutation symmetry. In physics, we call such particles **indistinguishable**.

Side note. *It turns out that the Hilbert space for any kind of bosons can be constructed in this manner, although the number of possible spins and the Hamiltonian may differ from those of photons. For fermions, we need to use a different kind of operators with a different algebra. The reverse strategy of constructing a quantum theory of fields from a theory of particles is sometimes called the second quantization (https://en.wikipedia.org/wiki/Second_quantization).*

Exercise 5.7. Find P_N and the wavefunctions $\{\psi_N\}$ for the coherent state $|\boldsymbol{\alpha}\rangle$.

Exercise 5.8. Let $\hat{a}_1$ be the annihilation operator for the mode with wavevector $\boldsymbol{k} = k\tilde{\boldsymbol{z}}$ and polarization vector

$$\tilde{\boldsymbol{e}}_1 \equiv \frac{\tilde{\boldsymbol{x}} + i\tilde{\boldsymbol{y}}}{\sqrt{2}}. \tag{5.90}$$

Let $\hat{a}_2$ be the annihilation operator for the mode with the same wavevector and polarization vector

$$\tilde{\boldsymbol{e}}_2 \equiv \frac{i\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{y}}}{\sqrt{2}}. \tag{5.91}$$

Let

$$|\text{Fock} : 1\rangle \equiv \hat{a}_1^\dagger |\text{vac}\rangle \,, \qquad\qquad |\text{Fock} : 2\rangle \equiv \hat{a}_2^\dagger |\text{vac}\rangle \,, \tag{5.92}$$

where we've omitted the wavevector for brevity.

(1) Show that $\tilde{\boldsymbol{e}}_1$ and $\tilde{\boldsymbol{e}}_2$ obey Eqs. (2.22)–(2.24).

(2) Show that $\{|\text{Fock} : 1\rangle \,, |\text{Fock} : 2\rangle\}$ are orthonormal if $[\hat{a}_j, \hat{a}_l] = 0$ and $[\hat{a}_j, \hat{a}_l^\dagger] = \delta_{jl}$.

(3) A new one-photon state is defined as

$$|\psi\rangle = \hat{b}^\dagger |\text{vac}\rangle = \cos\frac{\theta}{2} |\text{Fock} : 1\rangle + e^{i\phi} \sin\frac{\theta}{2} |\text{Fock} : 2\rangle \,, \tag{5.93}$$

where $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$. Find $\hat{b}$ in terms of $\hat{a}_1$ and $\hat{a}_2$ and find the polarization vector of the photon.

(4) A **Bloch sphere** is a representation of qubit states (https://en.wikipedia.org/wiki/Bloch_sphere). Each point on the sphere with spherical coordinates (θ, ϕ) represents a certain state $|\psi\rangle \langle\psi|$ with the θ and ϕ parameters.

Find the point on the Bloch sphere that represents a photon with each of the following polarizations:

$$\frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}} + i\tilde{\boldsymbol{y}}), \quad \frac{1}{\sqrt{2}}(i\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{y}}), \quad \tilde{\boldsymbol{x}}, \quad \tilde{\boldsymbol{y}}, \quad \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{y}}), \quad \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{x}} - \tilde{\boldsymbol{y}}). \tag{5.94}$$

Sketch your results by drawing a sphere and labeling each point with the polarization.

Exercise 5.9. Suppose that there are just two modes labeled by $j \in \{1, 2\}$ with annihilation operators $\hat{a}_1$ and $\hat{a}_2$, respectively. Suppose that a certain quantum state is expressed in the photon-number basis $\{|n_1, n_2\rangle : \text{each } n_j = 0, 1, 2, \dots\}$ as

$$|\psi\rangle = C_{2,0}\,|2,0\rangle + C_{1,1}\,|1,1\rangle + C_{0,2}\,|0,2\rangle\,, \qquad |C_{2,0}|^2 + |C_{1,1}|^2 + |C_{0,2}|^2 = 1. \tag{5.95}$$

Find the two-photon wavefunction $\psi_2(j, l)$ in terms of the C coefficients. Show explicitly that your result is symmetric, i.e.,

$$\psi_2(j, l) = \psi_2(l, j) \quad \text{for all } j, l, \tag{5.96}$$

and normalized, i.e.,

$$\sum_{j,l} |\psi_2(j, l)|^2 = 1. \tag{5.97}$$

Explain the physical meaning of $|C_{2,0}|^2$, $|C_{1,1}|^2$, and $|C_{0,2}|^2$. Explain the physical meaning of $|\psi_2(1, 1)|^2$, $|\psi_2(2, 2)|^2$, $|\psi_2(1, 2)|^2$, and $|\psi_2(2, 1)|^2$. You should find that

$$|C_{1,1}|^2 = |\psi_2(1, 2)|^2 + |\psi_2(2, 1)|^2. \tag{5.98}$$

Convince yourself that this is correct.

5.6.2. Continuum modes. Fock's method seems unnecessarily complicated for a discrete set of modes, since we could have just used the number states $\{|\boldsymbol{n}\rangle\}$, which form an orthonormal basis. When we have a continuum of modes, however, Fock's method is necessary if we want to write down an explicit construction of the Hilbert space.

We start by assuming that there is a vacuum state $|\text{vac}\rangle \in \mathcal{H}$ with $\langle\text{vac}|\text{vac}\rangle = 1$. In terms of the creation operators $\{\hat{a}^\dagger(\boldsymbol{k}, s)\}$, a Fock state is now defined as

$$\boxed{|\text{Fock} : j_1, \dots, j_N\rangle \equiv \frac{1}{\sqrt{N!}} \hat{a}^\dagger(\boldsymbol{k}_1, s_1) \dots \hat{a}^\dagger(\boldsymbol{k}_N, s_N)\,|\text{vac}\rangle\,,} \qquad \boxed{j_n \equiv (\boldsymbol{k}_n, s_n).} \tag{5.99}$$

The inner product between two of them becomes

$$\big\langle \text{Fock} : j_1, \dots, j_N \big| \text{Fock} : j'_1, \dots, j'_M \big\rangle = \frac{\delta_{NM}}{N!} \sum_{\mathcal{P}} \delta(j_1, j'_{\mathcal{P}(1)}) \dots \delta(j_1, j'_{\mathcal{P}(N)}), \tag{5.100}$$

$$\delta(j, j') \equiv \delta^3(\boldsymbol{k} - \boldsymbol{k}')\delta_{ss'}, \tag{5.101}$$

where

$$(\mathcal{P}(1), \dots, \mathcal{P}(N)) \tag{5.102}$$

is a permutation of $(1, \dots, N)$ and $\sum_{\mathcal{P}}$ is the sum over all $N!$ permutations. For example, if $N = 2$, then there are just $N! = 2$ permutations:

$$(\mathcal{P}(1), \mathcal{P}(2)) = (1, 2), \qquad (\mathcal{P}(1), \mathcal{P}(2)) = (2, 1), \tag{5.103}$$

and

$$\big\langle \text{Fock} : j_1, j_2 \big| \text{Fock} : j'_1, j'_2 \big\rangle = \frac{1}{2}\big[\delta(j_1, j'_1)\delta(j_2, j'_2) + \delta(j_1, j'_2)\delta(j_2, j'_1)\big] \tag{5.104}$$

$$= \frac{1}{2}\Big[\delta^3(\boldsymbol{k}_1 - \boldsymbol{k}'_1)\delta_{s_1 s'_1}\delta^3(\boldsymbol{k}_2 - \boldsymbol{k}'_2)\delta_{s_2 s'_2} + \delta^3(\boldsymbol{k}_1 - \boldsymbol{k}'_2)\delta_{s_1 s'_2}\delta^3(\boldsymbol{k}_2 - \boldsymbol{k}'_1)\delta_{s_2 s'_1}\Big]. \tag{5.105}$$

The completeness condition is now

$$\hat{I} = \sum_{N=0}^{\infty} \hat{\Pi}_N, \tag{5.106}$$

$$\hat{\Pi}_0 = |\text{vac}\rangle \langle \text{vac}|, \tag{5.107}$$

$$\hat{\Pi}_N = \sum_{s_1,\ldots,s_N} \int |\text{Fock} : j_1, \ldots, j_N\rangle \langle \text{Fock} : j_1, \ldots, j_N| \, d^3\boldsymbol{k}_1 \ldots d^3\boldsymbol{k}_N. \tag{5.108}$$

In quantum optics, Fock's method is useful when one needs to write down the quantum state for a continuum of modes, or when there are few photons. For example, under spontaneous parametric down-conversion (SPDC) in some crystal, the probability of generating $N > 2$ photons is negligible, and one can study the properties of the entangled photons via the two-photon wavefunction.

Exercise 5.10. Let a one-photon state be $\hat{b}_l^\dagger |\text{vac}\rangle$, where $\hat{b}_l$ is given by Eq. (3.115). Find the one-photon wavefunction $\psi_1(\boldsymbol{k}, s)$.

Exercise 5.11. Let the continuum displacement operator be

$$\hat{D}[\alpha] \equiv \exp\left[\sum_s \int \alpha(\boldsymbol{k}, s)\hat{a}^\dagger(\boldsymbol{k}, s)d^3\boldsymbol{k} - \text{H.c.}\right] |\text{vac}\rangle \tag{5.109}$$

and the coherent state be $|\alpha\rangle \equiv \hat{D}[\alpha] |\text{vac}\rangle$. Find $\{P_N\}$ and the wavefunctions $\{\psi_N\}$ defined as

$$\psi_N(j_1, \ldots, j_N) \equiv \frac{1}{\sqrt{P_N N!}} \langle \text{vac}| \, \hat{a}(\boldsymbol{k}_1, s_1) \ldots \hat{a}(\boldsymbol{k}_N, s_N) \, |\psi\rangle. \tag{5.110}$$

CHAPTER 6

Passive Linear Optics

6.1. Hamiltonian

Now that we have an idea of what quantum optical states look like, let's study dynamics. In optics, EM fields typically interact with matter so weakly that the equations of motion for the complex amplitudes are linear; we call such optical systems **linear optics**. Examples are many and include propagation in free space and in dielectric media, beam splitters, mirrors, polarizers, interferometers, optical fibers, optical resonators, etc. We see nonlinear optical effects only when the EM fields are very intense in matter that interacts strongly with them, e.g., with high-power lasers or in high-quality optical resonators. Linear optics forms a major part of optics.

The word "passive" refers to the fact that, apart from an initial state that is generated by some sources, the optics at zero temperature does not add photons to the EM fields. It will be easier to understanding what this means when we look at the Hamiltonian later.

In quantum optics, passive linear optics can be modeled by assuming that both the EM fields and the interacting matter consist of **coupled harmonic oscillators**. This is an approximation, as matter ultimately consists of atoms, electrons, nuclei, ions, etc. that are not exactly harmonic oscillators, but when the interactions are weak, the matter would behave effectively like harmonic oscillators when interacting with the EM fields. The best justification is perhaps the fact that the resulting equations of motion agree with those in classical optics.

Let's start with J EM modes. Assume that there are K other modes of harmonic oscillators in the matter that interact with the EM fields. Let

(1) $\{\hat{a}_j : j = 1, \ldots, J\}$ be the annihilation operators for **the EM modes** on Hilbert space $\mathcal{H}_{\text{EM}}$,

(2) $\{\hat{b}_j : j = 1, \ldots, K\}$ be the annihilation operators for **the matter modes** on Hilbert space $\mathcal{H}_{\text{matter}}$.

There are now $J + K$ modes, and we label the annihilation operators for all the modes by $\{\hat{c}_j\}$. Using matrix notation, we can write

$$\hat{\boldsymbol{c}} \equiv \begin{pmatrix} \hat{a}_1 \\ \vdots \\ \hat{a}_J \\ \hat{b}_1 \\ \vdots \\ \hat{b}_K \end{pmatrix} = \begin{pmatrix} \hat{\boldsymbol{a}} \\ \hat{\boldsymbol{b}} \end{pmatrix}, \qquad \hat{\boldsymbol{a}} \equiv \begin{pmatrix} \hat{a}_1 \\ \vdots \\ \hat{a}_J \end{pmatrix}, \qquad \hat{\boldsymbol{b}} \equiv \begin{pmatrix} \hat{b}_1 \\ \vdots \\ \hat{b}_K \end{pmatrix}, \tag{6.1}$$

so $\hat{\boldsymbol{c}}$ is a column vector of annhilation operators for the $J + K$ modes, the first J entries are for the EM modes, and the next K entries are for the matter modes. These modes don't need to be normal modes, but we still require them to satisfy the standard commutation relation

$$\boxed{[\hat{c}_j, \hat{c}_l^\dagger] = \delta_{jl}.} \tag{6.2}$$

When these modes may exchange particles with each other, a general Hamiltonian can be expressed as

$$\boxed{\hat{H} = \hbar \sum_{j,l} F_{jl} \hat{c}_j^\dagger \hat{c}_l,} \tag{6.3}$$

where F is a matrix with complex c-number entries called the coupling matrix. A derivation of this Hamiltonian from more physical assumptions will be given in Sec. 6.1.1 later, but for now we assume that Eq. (6.3) is given.

To see what the Hamiltonian does in the dynamics, let's look at the unitary operator with a tiny time step:

$$\hat{U}(\Delta t) = \exp\left(-i\sum_{j,l} F_{jl}\hat{c}_j^\dagger \hat{c}_l \Delta t\right) \approx \hat{I} - i\Delta t \sum_{j,l} F_{jl}\hat{c}_j^\dagger \hat{c}_l. \tag{6.4}$$

When this unitary is applied to a state $|\psi\rangle$, each $\hat{c}_l$ operator subtracts a boson from mode l, and then $\hat{c}_j^\dagger$ adds the boson to mode j. When the mode is EM, the bosons are, of course, photons, but when the mode is a matter mode, the bosons are stored physically as quanta of energy excitations in the matter; we just think of them as effective particles behaving like bosons and don't really care about them as much.

For longer times, remember that the unitary operator is just a product of the unitaries with tiny time steps ($\hat{U}(t) = \hat{U}(\Delta t)\ldots\hat{U}(\Delta t)$), so if we start with a definite total boson number, the total number of bosons in all the modes will stay constant. This behavior agrees with the observation that, at zero temperature (corresponding to the fact that the matter modes are in vacuum), many optical devices do not add photons to the EM fields (hence the word "passive").

Note that the optics may still take photons away and transfer them somewhere else to places we can't access. Thus, our model of passive linear optics can also model **optical loss**, which is physically the absorption of photons by matter; see Chapter 7 later.

For the fundamental principles of quantum mechanics to hold, the **Hamiltonian operator $\hat{H}$ must be Hermitian**. This means that the F matrix in Eq. (6.3) cannot be any matrix. Convince yourself that

$$\boxed{\hat{H} = \hat{H}^\dagger \quad \Leftrightarrow \quad F_{jl} = F_{lj}^*.} \tag{6.5}$$

In other words, **the F matrix must be Hermitian**.

Exercise 6.1. A fancier way of showing that the total photon number is conserved is to show that the total boson-number operator

$$\hat{N} \equiv \sum_j \hat{c}_j^\dagger \hat{c}_j \tag{6.6}$$

commutes with the unitary:

$$\left[\hat{U}, \hat{N}\right] = 0. \tag{6.7}$$

(1) Show that Eq. (6.7) holds if and only if

$$\hat{U}^\dagger \hat{N} \hat{U} = \hat{N}, \tag{6.8}$$

i.e., $\hat{N}$ is constant in the Heisenberg picture.

(2) If $|\psi_N\rangle$ is an eigenstate of $\hat{N}$, i.e.,

$$\hat{N}|\psi_N\rangle = N|\psi_N\rangle, \tag{6.9}$$

and Eq. (6.7) holds, show that $\hat{U}|\psi_N\rangle$ is also an eigenstate of $\hat{N}$ with the same eigenvalue N.

(3) If $\hat{U} = \exp\left(-\frac{i}{\hbar}\hat{H}t\right)$, it turns out that Eq. (6.7) holds if

$$[\hat{H}, \hat{N}] = 0. \tag{6.10}$$

Show that Eq. (6.10) holds, given Eqs. (6.3) and (6.6).

Exercise 6.2.

(1) Show that $\hat{H}$ can always be expressed as

$$\hat{H} = \hbar \sum_l \omega_l \hat{d}_l^\dagger \hat{d}_l \tag{6.11}$$

for some real numbers $\{\omega_l\}$, if $\hat{c}_j = \sum_l W_{jl}\hat{d}_l$ for some unitary matrix W_{jl}.

(2) Assume only two modes. Find $\{\omega_1, \omega_2\}$ and the W matrix if

$$F = \begin{pmatrix} \Omega - \Delta/2 & \kappa \\ \kappa^* & \Omega + \Delta/2 \end{pmatrix}. \tag{6.12}$$

(This exercise shows that, for passive linear optics, one can always define a set of normal modes, which oscillate in time simply as

$$\hat{d}_l(t) = \hat{d}_l \exp(-i\omega_l t) \tag{6.13}$$

in the Heisenberg picture. These normal modes are in general hybrid modes—each $\hat{d}_l(t) = \sum_j W^*_{jl}\hat{c}_j(t)$ is a combination of EM modes and matter modes oscillating together. The quanta associated with these normal modes are called **polaritons** [7]. The normal modes in dielectrics, optical fibers, dielectric resonators, etc., are polariton modes, strictly speaking; it's merely semantics whether we want to call them polaritons or photons.)

Side note. *In case you have seen papers talking about non-Hermitian Hamiltonians, they may refer to a few different things:*

*(1) Dynamics for **open quantum systems** interacting with an environment, in which case the evolution of a density operator is not described by a unitary operator but something more general (completely positive maps, master equations, etc.).*
*(2) Classical waves (e.g., classical optics) as mere **analogs** of quantum mechanics. Their "Hamiltonian" is not the Hamiltonian in quantum mechanics, just an analogous quantity. Fundamentally, the classical waves must still obey quantum mechanics, and a proper quantization of the classical theory is still needed. The true Hamiltonian must still be Hermitian.*
(3) Novel generalizations of quantum mechanics (even though we have zero experimental evidence so far that such generalizations are needed.)

For closed quantum systems, you'd break quantum mechanics if your Hamiltonian is not Hermitian (see Exercise 3.5), so you can't do that. Learn proper open quantum system theory before you attempt such a stunt.

6.1.1. Side note: Light-matter interaction. Here we go a little deeper into how Eq. (6.3) arises from a model of light-matter interactions by adopting an approach by Hopfield [8]. Suppose that the full Hamiltonian for light and matter is given by

$$\hat{H} = \hat{H}_{\text{matter}} + \hat{H}_{\text{EM}} + \hat{\eta}, \tag{6.14}$$

where $\hat{H}_{\text{matter}}$ is the matter Hamiltonian, $\hat{H}_{\text{EM}}$ is the Hamiltonian for the free EM fields, and

$$\hat{\eta} = -\iiint \hat{\boldsymbol{J}}(\boldsymbol{r}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{r}) d^3\boldsymbol{r} \tag{6.15}$$

models their interaction through the current density $\hat{\boldsymbol{J}}(\boldsymbol{r})$ and the vector potential $\hat{\boldsymbol{A}}$ given by Eq. (5.37). Just like how we quantize the EM fields, we may assume that the matter modes are a set of harmonic-oscillator modes with the Hamiltonian

$$\hat{H}_{\text{matter}} = \hbar \sum_l \omega'_l \hat{b}^\dagger_l \hat{b}_l, \tag{6.16}$$

where $\hat{b}_l$ is the annihilation operator of each matter normal mode and ω'_l is its natural frequency. The current density created by the matter may be written as

$$\hat{\boldsymbol{J}}(\boldsymbol{r}) = \sum_l \hat{b}_l \boldsymbol{w}_l(\boldsymbol{r}) + \text{H.c.}, \tag{6.17}$$

where $\boldsymbol{w}_l(\boldsymbol{r})$ is a mode function that expresses how each normal mode contributes to the current density, just like how the EM normal modes contribute to the EM fields $\hat{\boldsymbol{E}}$, $\hat{\boldsymbol{B}}$, and $\hat{\boldsymbol{A}}$.

Physically, the matter modes may arise from some kind of energy excitations, the quanta of which are often called quasiparticles. Examples include electron-hole pairs (excitons) and lattice vibrations (phonons). We would

need to go even deeper into the rabbit hole of condensed-matter physics, such as solid-state physics, to derive Eqs. (6.16) and (6.17). We won't do that here and take Eqs. (6.16) and (6.17) as given.

Given Eqs. (5.37) and (6.17), the interaction Hamiltonian given by Eq. (6.15) becomes a linear combination of the following two types of terms:

$$\hat{\eta} = -\iiint \hat{\boldsymbol{J}}(\boldsymbol{r}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{r}) d^3\boldsymbol{r} = \sum_{j,l} \left(C_{jl} \hat{a}_j^\dagger \hat{b}_l + \text{H.c.} \right) + \sum_{j,l} \left(D_{jl} \hat{a}_j \hat{b}_l + \text{H.c.} \right), \tag{6.18}$$

where C and D are matrices of constants. The first type of terms in the form of $\hat{a}_j^\dagger \hat{b}_l$ and $\hat{a}_j \hat{b}_l^\dagger$ are what we want and can be modeled by the passive-linear-optics Hamiltonian given by Eq. (6.3), while the second type in the form of $\hat{a}_j \hat{b}_l$ and $\hat{a}_j^\dagger \hat{b}_l^\dagger$ cannot be modeled by Eq. (6.3).

It turns out that the second type of terms can be thrown away if we make the so-called **rotating-wave approximation** (see Sec. D.5). We go to the **interaction picture**, where

$$\hat{\eta}_{\text{easy}}(t) = \sum_{j,l} \left[C_{jl} \hat{a}_j^\dagger \hat{b}_l e^{i(\omega_j - \omega_l')t} + \text{H.c.} \right] + \sum_{j,l} \left[D_{jl} \hat{a}_j \hat{b}_l e^{-i(\omega_j + \omega_l')t} + \text{H.c.} \right]. \tag{6.19}$$

In the rotating-wave approximation, we throw away terms that oscillate quickly in time in the Hamiltonian, because those terms average to zero over time and their net effects are negligible. So the $\hat{a}_j \hat{b}_l$ and $\hat{a}_j^\dagger \hat{b}_l^\dagger$ terms are thrown away, because they oscillate as $e^{\pm i(\omega_j + \omega_l')t}$. We may also throw away some of the $\hat{a}_j^\dagger \hat{b}_l$ and $\hat{a}_j \hat{b}_l^\dagger$ terms if $|\omega_j - \omega_l'|$ is large, keeping only the terms with $\omega_j - \omega_l' \approx 0$. In any case, we are left with the first type of terms in the form of $\hat{a}_j^\dagger \hat{b}_l$ and $\hat{a}_j \hat{b}_l^\dagger$. We may now go back to the Schrödinger picture, and the total Hamiltonian would be a linear combination of only terms in the form of

$$\hat{a}_j^\dagger \hat{a}_j, \quad \hat{b}_l^\dagger \hat{b}_l, \quad \hat{a}_j^\dagger \hat{b}_l, \quad \hat{a}_j \hat{b}_l^\dagger, \tag{6.20}$$

so that the Hamiltonian can be written in the form of Eq. (6.3).

6.2. Heisenberg picture

With the Hamiltonian given by Eq. (6.3), the equations of motion for each $\hat{c}_j(t)$ in the Heisenberg picture is simple to derive. Let

$$\hat{c}_j(t) \equiv \hat{U}^\dagger(t) \hat{c}_j \hat{U}(t). \tag{6.21}$$

Then the Heisenberg equations become

$$\frac{d\hat{c}_j(t)}{dt} = -i \sum_l F_{jl} \hat{c}_l(t). \tag{6.22}$$

If we think of $\hat{\boldsymbol{c}}(t)$ as a column vector of annihilation operators, then we can also rewrite Eq. (6.22) in matrix notation:

$$\boxed{\frac{d\hat{\boldsymbol{c}}(t)}{dt} = -iF\hat{\boldsymbol{c}}(t),} \tag{6.23}$$

where $F\hat{\boldsymbol{c}}(t)$ is understood as the matrix F applied to the column vector $\hat{\boldsymbol{c}}(t)$.

The Heisenberg-picture equations are linear and agree with what we know about passive linear optics in classical optics. The $\hat{\boldsymbol{b}}$ operators play the same role as the polarization field $\boldsymbol{P}(\boldsymbol{r}, t)$ in classical EM; see Appendix F for a quick review. The new restriction imposed by the quantum treatment is that the matrix F must be Hermitian.

The general solution of Eq. (6.23) is simple to write down:

$$\boxed{\hat{\boldsymbol{c}}(t) = \exp(-iFt)\hat{\boldsymbol{c}}(0).} \tag{6.24}$$

where $\exp(-iFt)$ is interpreted as the exponential of a matrix. We know from linear algebra that, since F is Hermitian, $\exp(-iFt)$ must be a unitary matrix. Let's call the unitary matrix V, so that we can write

$$\boxed{\hat{\boldsymbol{c}}(t) = V(t)\hat{\boldsymbol{c}}(0),} \tag{6.25}$$

$$\boxed{V(t) \equiv \exp(-iFt).} \tag{6.26}$$

This result agrees with the classical **coupled-mode equations** for passive linear optics. In practice, we can often just take the matrix $V(t)$ from classical optics and plug it in Eq. (6.25), without redoing the quantum derivation. We should make sure that $V(t)$ is a unitary matrix, however, so that we don't break quantum mechanics.

With a unitary V, you can verify the general fact that the entries of $\hat{\boldsymbol{c}}(t)$ still obey the fundamental commutation relation

$$\boxed{[\hat{c}_j(t), \hat{c}_l^\dagger(t)] = \delta_{jl},} \tag{6.27}$$

which must hold for any dynamics in general, not just passive linear optics, so we are assured that we haven't made any mistake.

The Heisenberg picture is convenient for computing expected values. For example, given Eq. (6.25), we know $\hat{c}_j(t) = \sum_l V_{jl}(t)\hat{c}_l$, so the average amplitude of mode j at time t given an initial state $|\psi\rangle$ (which doesn't change in time in the Heisenberg picture) is

$$\langle\psi|\, \hat{c}_j(t)\, |\psi\rangle = \sum_l V_{jl}(t)\, \langle\psi|\, \hat{c}_l\, |\psi\rangle\,, \tag{6.28}$$

while the expected boson number in mode j at time t is

$$\langle\psi|\, \hat{c}_j^\dagger(t)\hat{c}_j(t)\, |\psi\rangle = \sum_{l,m} V_{jl}^*(t)V_{jm}(t)\, \langle\psi|\, \hat{c}_l^\dagger\hat{c}_m\, |\psi\rangle\,, \tag{6.29}$$

where $\langle\psi|\, \hat{c}_l\, |\psi\rangle$ and $\langle\psi|\, \hat{c}_l^\dagger\hat{c}_m\, |\psi\rangle$ are determined by the initial state $|\psi\rangle$.

Exercise 6.3. Verify Eq. (6.22).

Exercise 6.4. Derive Eq. (6.27) from Eq. (6.21) for any unitary $\hat{U}(t)$. Also derive Eq. (6.27) independently from Eq. (6.25), to show that the V matrix must be unitary.

Exercise 6.5. Find the $V(t)$ matrix if there are only EM normal modes.

Exercise 6.6. Suppose that we redefine the $J + K$ modes using a unitary W matrix:

$$\hat{c}_j = \sum_l W_{jl}\hat{d}_l, \qquad\qquad \hat{d}_l = \sum_j W_{jl}^*\hat{c}_j. \tag{6.30}$$

(1) Show that the Hamiltonian given by Eq. (6.3) becomes

$$\hat{H} = \hbar\sum_{j,l} F'_{jl}\hat{d}_j^\dagger\hat{d}_l, \tag{6.31}$$

which has the same form as Eq. (6.3) but with a new coupling matrix F'. Find F' in terms of the old F and prove that F' remains Hermitian if F is Hermitian and W is unitary.

(2) Given Eq. (6.25), show that the Heisenberg equations of motion for $\hat{d}_j(t)$ can also be written as

$$\hat{d}_j(t) = \sum_l V'_{jl}(t)\hat{d}_l(0), \tag{6.32}$$

where V' is another matrix you should find in terms of F'. Find also V' in terms of V and W. Show that the V' in terms of V and W is also unitary.

(This exercise is important because it shows us that passive linear optics has the same form of Hamiltonian and the same form of equations of motion regardless of how the modes are defined, as long as they are related to the original ones by a unitary matrix W.)

6.3. Example: pulse propagation in free space

With only EM fields in free space, we don't have matter modes to worry about, and we know that normal sinusoidal modes have annihilation operators that obey $\hat{a}_j(t) = \hat{a}_j \exp(-i\omega_j t)$ in the Heisenberg picture. In practice, we don't often deal with sinusoidal modes directly, however, and sources and detectors may be more conveniently modeled using some other set of modes, e.g., optical pulses, which will behave like the coupled oscillators that we studied in Sec. 3.5.

Let the annihilation operator of a new mode labeled by l be

$$\hat{f}_l = \sum_j W_{jl}^* \hat{a}_j, \tag{6.33}$$

where $\{\hat{a}_j\}$ are the operators for the sinusoidal modes. Recall from Sec. 3.5.2 that such a new mode has an electric field that is a superposition of sinusoidal waves, and W_{jl} as a function of $j = (\boldsymbol{k}, s)$ is called the $(\boldsymbol{k}, s)$-space amplitude that determines the weight of each sinusoidal wave in the new mode. In the Heisenberg picture,

$$\hat{f}_l(t) \equiv \hat{U}^\dagger(t)\hat{f}_l\hat{U}(t) = \sum_j W_{jl}^* \hat{U}^\dagger(t)\hat{a}_j\hat{U}(t) = \sum_j W_{jl}^* e^{-i\omega_j t}\hat{a}_j = \sum_j \left(W_{jl}e^{i\omega_j t}\right)^* \hat{a}_j \tag{6.34}$$

We see that $\hat{f}_l(t)$ has the same form as Eq. (6.33), except that it is the annihilation operator for another mode, with a $(\boldsymbol{k}, s)$-space amplitude given by $W_{jl}e^{i\omega_j t}$.

To be more specific, let's follow the optical-pulse example in Sec. 3.5.2 and write

$$W_{jl} = \delta_{s1}\delta_{k_x 0}\delta_{k_y 0} g(k_z) \exp(-ik_z z_l), \tag{6.35}$$

so that the pulse mode consists of sinusoidal waves with one polarization $s = 1$, $k_x = 0$, and $k_y = 0$ only. $g(k_z)$ governs the weight of each sinusoidal wave with a certain value of k_z in the pulse mode. g can be the rectangle function assumed in Sec. 3.5.2, or any function in general, e.g., Gaussian, but keep in mind that we'll often assume that $g(k_z)$ is highly concentrated near some wavenumber $k_z = k_0$ that is close to an optical value, as shown in Fig. 6.1. Recall that, because of the phase factor $\exp(-ik_z z_l)$, this mode has an electric field that looks like **a pulse centered at** $z = z_l$. For clarity, I will rewrite $\hat{f}_l(t)$ as

$$\hat{f}_l(t) = \hat{f}(z_l, t) = \sum_j \left(W_{jl}e^{i\omega_j t}\right)^* \hat{a}_j, \tag{6.36}$$

to show explicitly the dependence of $\hat{f}_l(t)$ on z_l. For example, $\hat{f}(z_l, 0)$ is just

$$\hat{f}(z_l, 0) = \hat{f}_l(0) = \hat{f}_l = \sum_j W_{jl}^* \hat{a}_j. \tag{6.37}$$

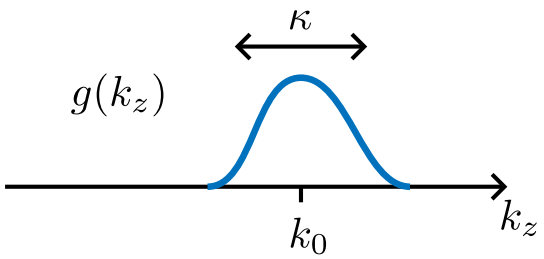

FIGURE 6.1. A sketch of a typical $g(k_z)$ function.

Suppose that $g(k_z) = 0$ for $k_z < 0$, so that we have a superposition of sinusoidal waves with positive k_z only. Then ω_j can be expressed as

$$\omega_j = \omega_{\boldsymbol{k}} = c|k_z| = ck_z. \tag{6.38}$$

The $(\boldsymbol{k}, s)$-space amplitude of $\hat{f}(z_l, t)$ in Eq. (6.36) becomes

$$W_{jl}e^{i\omega_j t} = \delta_{k_x 0}\delta_{k_y 0}\delta_{s1}g(k_z)\exp(-ik_z z_l)\exp(ick_z t) \tag{6.39}$$

$$= \delta_{k_x 0}\delta_{k_y 0}\delta_{s1}g(k_z)\exp[-ik_z(z_l - ct)]. \tag{6.40}$$

This looks very much like the W_{jl} given by Eq. (6.35) for the initial $\hat{f}(z_l, 0)$ in Eq. (6.37), except that z_l is replaced by $z_l - ct$. In other words, $W_{jl}e^{i\omega_j t}$ is the $(\boldsymbol{k}, s)$-space amplitude of a pulse **centered at** $z = z_l - ct$. Hence, we can write

$$\boxed{\hat{f}(z_l, t) = \hat{f}(z_l - ct, 0).} \tag{6.41}$$

You may have seen this sort of solution to 1D pulse propagation in classical optics, but the precise physical meaning of the Heisenberg picture is rather obscure. For example, suppose we'd like to compute the average amplitude of the pulse mode centered at z_l at time t. This average amplitude is given by

$$\langle\psi|\,\hat{f}(z_l, t)\,|\psi\rangle = \langle\psi|\,\hat{f}(z_l - ct, 0)\,|\psi\rangle\,. \tag{6.42}$$

Recall that $|\psi\rangle$ is the state at $t = 0$ and it doesn't change in the Heisenberg picture. This expression means that the average amplitude of the pulse mode centered at z_l at time t is equal to the average amplitude of the pulse mode centered at $z_l - ct$ at time 0.

In general, Eq. (6.41) implies that, if we measure the pulse mode centered at z_l at time t, it is as if we apply the same measurement to the pulse mode centered at $z_l - ct$ at time 0; the probability distributions will be exactly the same. See Fig. 6.2 for an illustration.

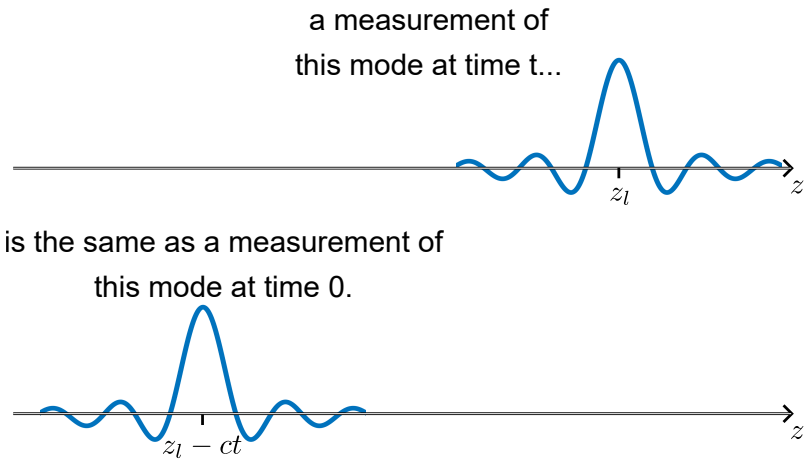

FIGURE 6.2. An interpretation of the Heisenberg picture for pulse propagation.

This result agrees with the classical picture that a pulse propagates from position $z_l - ct$ to position z_l after time t, even though the precise physical interpretation of the Heisenberg picture is a bit hard to comprehend.

6.4. A sequence of pulses

Instead of thinking about one pulse mode at one time, imagine a detector that sits at one position, say, z_0, and just waits for the pulses to come to it. Then the detector can measure multiple pulse modes over time. For example, at $t = 0$, we have

$$\hat{f}(z_0, 0) = \hat{f}(z_0, 0), \tag{6.43}$$

at $t = \Delta t$, we have

$$\hat{f}(z_0, \Delta t) = \hat{f}(z_0 - c\Delta t, 0), \tag{6.44}$$

which corresponds to a different pulse mode, and at $t = 2\Delta t$, we have

$$\hat{f}(z_0, 2\Delta t) = \hat{f}(z_0 - 2c\Delta t, 0), \tag{6.45}$$

which is yet another pulse mode, and so on and so forth. Measurements at z_0 of the pulses that come to the detector one by one over time is equivalent to a measurement of all the pulse modes at one time 0; Fig. 6.3 offers an illustration. The former is how we measure pulses in practice, so it is more common in optics to write the pulse-mode operators as

$$\hat{f}(z_0, 0), \hat{f}(z_0, \Delta t), \hat{f}(z_0, 2\Delta t), \ldots \tag{6.46}$$

at one position z_0 and multiple times, rather than

$$\hat{f}(z_0, 0), \hat{f}(z_1, 0), \hat{f}(z_2, 0), \ldots \tag{6.47}$$

at one time and multiple positions.

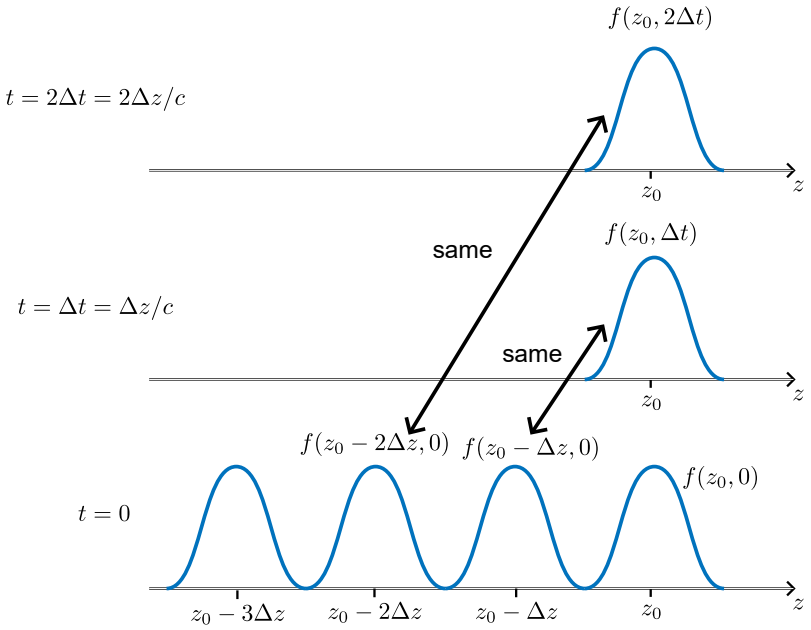

FIGURE 6.3. Multiple pulse modes can be measured by sitting at one position z_0 and wait for the pulses to come.

If the pulse modes satisfy the usual commutation relations

$$[\hat{f}(z_l, 0), \hat{f}(z_m, 0)] = 0, \qquad [\hat{f}(z_l, 0), \hat{f}^\dagger(z_m, 0)] = \delta_{lm} \tag{6.48}$$

for different positions at the same time, and we set

$$z_l = z_0 + l\Delta z, \qquad \Delta t = \frac{\Delta z}{c}, \tag{6.49}$$

so that Δz is the distance between adjacent pulses, then we can write

$$\hat{f}(z_0, t_m) = \hat{f}(z_0 - ct_m, 0) = \hat{f}(z_0 - m\Delta z, 0), \quad t_m \equiv m\Delta t, \quad m \text{ is an integer}, \tag{6.50}$$

and obtain the following commutation relations for the operators at different times:

$$\boxed{\left[\hat{f}(z_0, t_m), \hat{f}(z_0, t_n)\right] = 0,} \qquad \boxed{\left[\hat{f}(z_0, t_m), \hat{f}^\dagger(z_0, t_n)\right] = \delta_{mn}.} \tag{6.51}$$

At the end of the day, this is just a different convention of writing the operators for a sequence of pulse modes, to make them look more like the convention in optics, where pulses are described and measured in the time domain instead of the space domain.

For each pulse mode, it is also customary to describe its electric field in terms of time-domain quantities rather than the space-domain quantities we assumed in Sec. 3.5.2. The translation is as follows:

(1) The rapid oscillation term $\exp(ik_0 z)$ for a pulse becomes $\exp[ik_0(z-ct)]$ if we sit at one place and measure the electric field in time, so ck_0 is the frequency (in radian/s) of the oscillation in time.
(2) The spectrum of the pulse as a function of ω (frequency in radian/s) becomes $g(\omega/c)$, where we replace k_z by ω/c. For example, for the rectangle example in Sec. 3.5.2,

$$g(k_z) \propto \text{rect}\left(\frac{k_z - k_0}{\kappa}\right), \qquad g(\omega/c) = \text{rect}\left(\frac{\omega - ck_0}{c\kappa}\right), \tag{6.52}$$

so the center frequency of the spectrum in ω domain becomes

$$\omega_0 \equiv ck_0, \tag{6.53}$$

and the bandwidth of the spectrum becomes $c\kappa$.
(3) The pulse width in time domain is now $\propto 1/(c\kappa)$.
(4) Instead of using Δz to describe the distance between adjacent pulses in space, we use $\Delta t = \Delta z/c$ to describe the spacing in time.

To give some typical numbers, if the center spatial frequency is $k_0 = 2\pi/\lambda_0$, where $\lambda_0 = 1550$ nm (typical wavelength for optical fiber communications), then $ck_0 \approx 2\pi \times 200$ THz (1 THz (Tera-Hertz) is 10^{12} Hz). If $\Delta t = 1$ ns, then the pulse repetition rate would be $1/\Delta t = 1$ GHz.

6.5. Schrödinger picture

Advantages of the Heisenberg picture:

(1) The equations of motion are simple, at least for passive linear optics.
(2) They look exactly like those in classical optics.

Disadvantages:

(1) The precise physical meaning is rather obscure.
(2) Many other subjects in quantum physics, such as quantum information and open quantum system theory, use the Schrödinger picture almost exclusively, so it's hard to relate any Heisenberg-picture result to those subjects.

To adopt the Schrödinger picture, we need to compute $\hat{U}(t)\,|\psi\rangle$. This is often possible for passive linear optics and special initial states, by leveraging the simple math from the Heisenberg picture.

6.5.1. Coherent states. For an initial coherent state, we can take advantage of its definition in terms of the displacement operator to write

$$\hat{U}(t)\,|\boldsymbol{\alpha}\rangle = \hat{U}(t)\hat{D}(\boldsymbol{\alpha})\,|\text{vac}\rangle = \hat{U}(t)\hat{D}(\boldsymbol{\alpha})\hat{U}^\dagger(t)\hat{U}(t)\,|\text{vac}\rangle\,. \tag{6.54}$$

$\hat{D}(\boldsymbol{\alpha})$ is now expressed in terms of the $\hat{\boldsymbol{c}}$ operators, i.e.,

$$\hat{D}(\boldsymbol{\alpha}) = \exp\left[\sum_j \alpha_j \hat{c}_j^\dagger - \text{H.c.}\right]. \tag{6.55}$$

(I could have written it as $\hat{D}(c:\boldsymbol{\alpha})$ but I won't, for brevity.) For passive linear optics, it can be shown that

$$\hat{U}(t)\,|\text{vac}\rangle = |\text{vac}\rangle\,. \tag{6.56}$$

Then we need to compute $\hat{U}(t)\hat{D}(\boldsymbol{\alpha})\hat{U}^\dagger(t)$. Using Eq. (B.76), we find that

$$\hat{U}(t)\hat{D}(\boldsymbol{\alpha})\hat{U}^\dagger(t) = \exp\left[\sum_j \alpha_j \hat{U}(t)\hat{c}_j^\dagger\hat{U}^\dagger(t) - \text{H.c.}\right]. \tag{6.57}$$

We also know

$$\hat{U}(t) = \hat{U}^\dagger(-t), \tag{6.58}$$

so $\hat{U}(t)\hat{c}_j^\dagger\hat{U}^\dagger(t) = \hat{U}^\dagger(-t)\hat{c}_j^\dagger\hat{U}(-t)$ is just the Heisenberg picture of $\hat{c}_j^\dagger$ with negative time. We can then take advantage of the Heisenberg-picture result given by Eq. (6.25) to find

$$\hat{U}(t)\hat{c}_j^\dagger\hat{U}^\dagger(t) = \hat{U}^\dagger(-t)\hat{c}_j^\dagger\hat{U}(-t) = \sum_l V_{jl}^*(-t)\hat{c}_l^\dagger. \tag{6.59}$$

Notice that the matrix $V(t)$ obeys $V^\dagger(t) = \exp(iFt) = V(-t)$, so

$$V_{jl}^*(-t) = [V^\dagger(-t)]_{lj} = [V(t)]_{lj} = V_{lj}(t). \tag{6.60}$$

Hence

$$\hat{U}(t)\hat{c}_j^\dagger\hat{U}^\dagger(t) = \sum_l V_{lj}(t)\hat{c}_l^\dagger, \tag{6.61}$$

$$\hat{U}(t)\hat{D}(\boldsymbol{\alpha})\hat{U}^\dagger(t) = \exp\left[\sum_{j,l}\alpha_j V_{lj}(t)\hat{c}_l^\dagger - \text{H.c.}\right]. \tag{6.62}$$

This is still a displacement operator, but now the complex amplitude in front of each $\hat{c}_l^\dagger$ becomes

$$\sum_j V_{lj}(t)\alpha_j. \tag{6.63}$$

Hence

$$\hat{U}(t)\hat{D}(\boldsymbol{\alpha})\hat{U}^\dagger(t) = \hat{D}(V(t)\boldsymbol{\alpha}), \tag{6.64}$$

$$\boxed{\hat{U}(t)\left|\boldsymbol{\alpha}\right\rangle = \left|V(t)\boldsymbol{\alpha}\right\rangle.} \tag{6.65}$$

This is a neat result, because it says that, in the Schrödinger picture, a coherent state remains a coherent state, and its amplitude $\boldsymbol{\alpha}$ evolves as $V(t)\boldsymbol{\alpha}$, just like the equation of motion given by Eq. (6.25) and just like classical optics. This result is a lot more intuitive than the Heisenberg picture, although it is specific to a coherent state.

Exercise 6.7. Verify Eq. (6.56).

Exercise 6.8. Assume that $\{\hat{a}_j\}$ are annihilation operators of normal sinusoidal modes with $j = (\boldsymbol{k}, s)$. Let the amplitude of a coherent state in the $(\boldsymbol{k}, s)$ space at time $t = 0$ be

$$\alpha_j \propto \delta_{s1}\delta_{k_x 0}\delta_{k_y 0}g(k_z)\exp(-ik_z z_1). \tag{6.66}$$

In other words, the excited mode of the coherent state is initially an optical pulse centered at $z = z_1$. Assume that $g(k_z) = 0$ for $k_z < 0$. Find $\hat{U}(t)\left|\boldsymbol{\alpha}\right\rangle$ and show that the excited mode of the coherent state at time t is an optical pulse centered at $z = z_1 + ct$, as illustrated in Fig. 6.4.

6.5.2. Sudarshan representation. Now we can exploit the simple result for a coherent state to study the Schrödinger picture of an arbitrary density operator in terms of the Sudarshan representation in Sec. 5.4. Suppose that the initial state is $\hat{\rho}$, with a Sudarshan representation given by $\Phi(\boldsymbol{\alpha})$. Then the Schrödinger-picture density operator with passive linear optics becomes

$$\hat{\rho}(t) \equiv \hat{U}(t)\hat{\rho}\hat{U}^\dagger(t) = \int \Phi(\boldsymbol{\alpha})\hat{U}(t)\left|\boldsymbol{\alpha}\right\rangle\left\langle\boldsymbol{\alpha}\right|\hat{U}^\dagger(t)d^{2J}\boldsymbol{\alpha} = \boxed{\int \Phi(\boldsymbol{\alpha})\left|V(t)\boldsymbol{\alpha}\right\rangle\left\langle V(t)\boldsymbol{\alpha}\right| d^{2J}\boldsymbol{\alpha}.} \tag{6.67}$$

If Φ is nonnegative, we can again think of this state as a noisy coherent state, the amplitude $\boldsymbol{\alpha}$ as a classical random variable, and $\Phi(\boldsymbol{\alpha})$ as the probability density of the random variable at initial time. But bear in mind that Eq. (6.67) works for any Φ in general, and we shall see that the Sudarshan representation is quite handy in derivations involving passive linear optics.

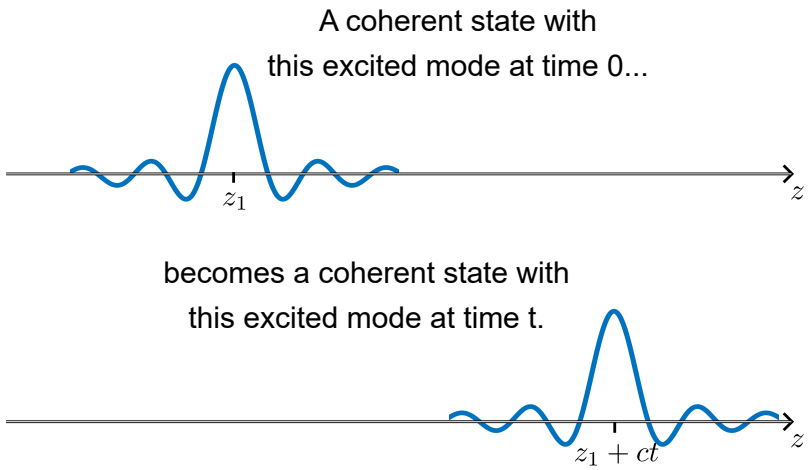

FIGURE 6.4. Schrödinger picture of a coherent state when the excited mode is a pulse.

Exercise 6.9. Show that Eq. (6.67) can also be expressed as

$$\hat{\rho}(t) = \int \Phi(V^\dagger(t)\boldsymbol{\beta})\,|\boldsymbol{\beta}\rangle\,\langle\boldsymbol{\beta}|\,d^{2J}\boldsymbol{\beta}. \tag{6.68}$$

Hint: you can assume the fact

$$d^{2J}\boldsymbol{\beta} \equiv \prod_{j=1}^{J}(d\,\mathrm{Re}\,\beta_j)(d\,\mathrm{Im}\,\beta_j) = d^{2J}\boldsymbol{\alpha} \tag{6.69}$$

if $\boldsymbol{\beta} = V\boldsymbol{\alpha}$ and V is a unitary matrix.

6.5.3. Fock representation. For an arbitrary pure state, we can still make some progress if we use the Fock representation. For a discrete set of modes, the Fock representation of any state is given by Eq. (5.82). The Schrödinger picture of the state becomes

$$\hat{U}(t)\,|\psi\rangle = \sum_{N=0}^{\infty}\sum_{\boldsymbol{j}\in\{1,\ldots,J\}^N} |\text{Fock} : \boldsymbol{j}\rangle\,\langle\text{Fock} : \boldsymbol{j}|\,\hat{U}(t)\,|\psi\rangle\,. \tag{6.70}$$

The N-boson wavefunction can be expressed as

$$\langle\text{Fock} : \boldsymbol{j}|\,\hat{U}(t)\,|\psi\rangle = \frac{1}{\sqrt{N!}}\,\langle\text{vac}|\,\hat{c}_{j_1}\ldots\hat{c}_{j_N}\hat{U}(t)\,|\psi\rangle\,. \tag{6.71}$$

If we insert $\hat{U}(t)\hat{U}^\dagger(t)$ in front of each $\hat{c}_{j_n}$, we find

$$\langle\text{Fock} : \boldsymbol{j}|\,\hat{U}(t)\,|\psi\rangle = \frac{1}{\sqrt{N!}}\underbrace{\langle\text{vac}|\,\hat{U}(t)}_{\langle\text{vac}|}\underbrace{\hat{U}^\dagger(t)\hat{c}_{j_1}\hat{U}(t)}_{\hat{c}_{j_1}(t)}\underbrace{\hat{U}^\dagger(t)\hat{c}_{j_2}\hat{U}(t)}_{\hat{c}_{j_2}(t)}\ldots\underbrace{\hat{U}^\dagger(t)\hat{c}_{j_N}\hat{U}(t)}_{\hat{c}_{j_N}(t)}\,|\psi\rangle\,. \tag{6.72}$$

It can be shown that $\langle\text{vac}|\,\hat{U}(t) = \langle\text{vac}|$. We can also exploit the Heisenberg-picture result given by Eq. (6.25) once again to find that $\hat{U}^\dagger(t)\hat{c}_j\hat{U}(t) = \hat{c}_j(t) = \sum_l V_{jl}(t)\hat{c}_l$, leading to

$$\langle\text{Fock} : \boldsymbol{j}|\,\hat{U}(t)\,|\psi\rangle = \sum_{l_1,\ldots,l_N} V_{j_1 l_1}(t)\ldots V_{j_N l_N}(t)\frac{1}{\sqrt{N!}}\,\langle\text{vac}|\,\hat{c}_{l_1}\ldots\hat{c}_{j_l}\,|\psi\rangle \tag{6.73}$$

$$= \boxed{\sum_{l_1,\ldots,l_N} V_{j_1 l_1}(t)\ldots V_{j_N l_N}(t)\,\langle\text{Fock} : \boldsymbol{l}|\psi\rangle\,.} \tag{6.74}$$

$\langle \text{Fock} : \boldsymbol{l}|\psi\rangle$ is the N-photon wavefunction at $t = 0$ (unnormalized). We may think of $V_{j_1 l_1} \dots V_{j_N l_N}$ as a Green's function $G(\boldsymbol{j}, t|\boldsymbol{l}, 0)$, also called a propagator:

$$\langle \text{Fock} : \boldsymbol{j}| \hat{U}(t) |\psi\rangle = \sum_{\boldsymbol{l}} G(\boldsymbol{j}, t|\boldsymbol{l}, 0) \langle \text{Fock} : \boldsymbol{l}|\psi\rangle , \tag{6.75}$$

$$G(\boldsymbol{j}, t|\boldsymbol{l}, 0) = V_{j_1 l_1}(t) \dots V_{j_N l_N}(t). \tag{6.76}$$

In particular, when there is only one boson ($N = 1$),

$$G(\boldsymbol{j}, t|\boldsymbol{l}, 0) = V_{j_1 l_1}(t), \tag{6.77}$$

so we can call V the one-particle propagator. For N bosons in passive linear optics, the total propagator is simply a product of one-particle propagators.

For example, suppose that the initial wavefunction is a product of one-particle functions:

$$\langle \text{Fock} : \boldsymbol{l}|\psi\rangle \propto \phi(l_1) \dots \phi(l_N). \tag{6.78}$$

We may interpret this as a wavefunction of **independent** bosons, since the probability density $\propto |\phi(l_1) \dots \phi(l_N)|^2$ is that of independent random variables. In particular, a coherent state gives such wavefunctions for all N (Exercise 5.7). Then

$$\langle \text{Fock} : \boldsymbol{j}| \hat{U}(t) |\psi\rangle = \left[\sum_{l_1} V_{j_1 l_1}(t)\phi(l_1)\right] \dots \left[\sum_{l_N} V_{j_N l_N}(t)\phi(l_N)\right]. \tag{6.79}$$

Each one-particle function $\phi(l_n)$ simply evolves on its own, the wavefunction remains a product of one-particle functions, and the bosons at any time remain independent from one another.

Passive linear optics in the Fock representation resembles a model of bosons that do not interact with one another. But it is important that we do not confuse this particle picture with the oscillator picture, where the oscillators are coupled by passive linear optics.

6.6. Example: lossless beam splitter

A beam splitter is a basic workhorse in passive linear optics (https://en.wikipedia.org/wiki/Beam_splitter). It is used typically with two input optical beams aligned carefully so that they meet at the beam splitter and produce two output optical beams, as depicted in Fig. 6.5.

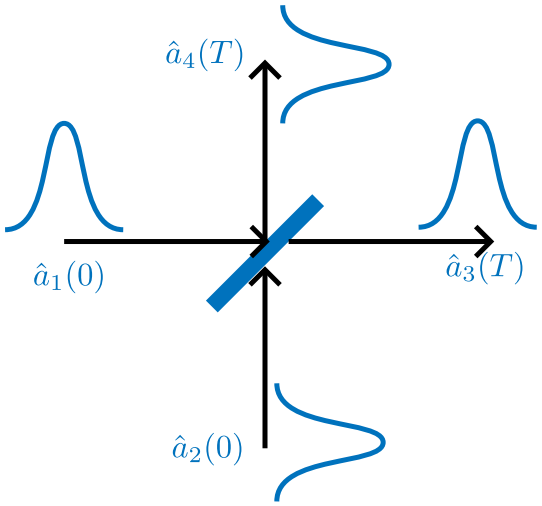

FIGURE 6.5. An illustration of a beam splitter.

6.6.1. Heisenberg picture. Suppose that we measure a pulse mode at time T in each of the two output beams. Let the Heisenberg-picture annihilation operators be $\hat{a}_3(T)$ and $\hat{a}_4(T)$, respectively. The interaction between all the EM modes and the matter modes in the beam splitter is in general quite complicated, and the two operators would depend on all the other modes:

$$\hat{a}_3(T) = V_{31}(T)\hat{a}_1(0) + V_{32}(T)\hat{a}_2(0) + \dots, \tag{6.80}$$

$$\hat{a}_4(T) = V_{41}(T)\hat{a}_1(0) + V_{42}(T)\hat{a}_2(0) + \dots. \tag{6.81}$$

Instead of deriving the V matrix from first principles, we cheat a little bit by peeking at classical optics and ask how we can make our equations of motion consistent with it.

Let $\alpha_3(T)$ and $\alpha_4(T)$ be the c-number amplitudes of those output pulse modes in classical optics. For a beam splitter, they can be expressed in terms of the c-number amplitudes for two input pulse modes, denoted as $\alpha_1(0)$ and $\alpha_2(0)$, like this:

$$\begin{pmatrix}\alpha_3(T)\\ \alpha_4(T)\end{pmatrix} = \underbrace{\begin{pmatrix}\tau & r\\ r' & \tau'\end{pmatrix}}_{\equiv S}\begin{pmatrix}\alpha_1(0)\\ \alpha_2(0)\end{pmatrix}, \tag{6.82}$$

where τ, τ' are the transmission coefficients of the beam splitter and r', r' are the reflection coefficients (all complex numbers). This relation is called an **input-output relation** and the S matrix is called **the scattering matrix**. There may be many modes in the problem, but at a certain time T and for the output pulse modes we are looking at, the two output amplitudes $\alpha_{3,4}(T)$ depend on only two input amplitudes $\alpha_{1,2}(0)$:

(1) $\alpha_3(T) = \tau\alpha_1(0) + r\alpha_2(0)$ means that the output is a superposition of two contributions: the first input $\alpha_1(0)$ multiplied by a transmission coefficient τ, and the second input $\alpha_2(0)$ multiplied by a reflection coefficient r.

(2) $\alpha_4(T) = r'\alpha_1(0) + \tau'\alpha_2(0)$ means that the output is a superposition of the first input $\alpha_1(0)$ multiplied by a reflection coefficient r' and the second input $\alpha_2(0)$ multiplied by a transmission coefficient τ'.

For our quantum equations to be consistent with the classical ones, they should obey

$$\langle\psi|\,\hat{a}_j(T)\,|\psi\rangle = \alpha_j(T). \tag{6.83}$$

Eqs. (6.80) and (6.81) can be made to give the classical Eq. (6.82) if we set

$$\begin{pmatrix}V_{31}(T) & V_{32}(T)\\ V_{41}(T) & V_{42}(T)\end{pmatrix} = S = \begin{pmatrix}\tau & r\\ r' & \tau'\end{pmatrix}, \tag{6.84}$$

$$V_{3j}(T) = 0 \text{ and } V_{4j}(T) = 0 \quad \text{for } j = 3, 4, \dots, \tag{6.85}$$

so that $\hat{a}_3(T)$ and $\hat{a}_4(T)$ depend only on $\hat{a}_1(0)$ and $\hat{a}_2(0)$ and not the other $\hat{a}_j(0)$'s. We obtain

$$\boxed{\begin{pmatrix}\hat{a}_3(T)\\ \hat{a}_4(T)\end{pmatrix} = S\begin{pmatrix}\hat{a}_1(0)\\ \hat{a}_2(0)\end{pmatrix},} \tag{6.86}$$

the averages of which agree with the classical Eq. (6.82).

This method seems quick and dirty, so we should double-check that everything remains legal in the quantum case. Remember that, in the quantum case, the big V matrix must be unitary. Then Eq. (6.85) holds and we have only two inputs and two outputs if and only if **the scattering matrix S is unitary** (see Exercise 6.10). This is called the **lossless assumption**. To reassure ourselves, we can double-check that, given a unitary S, the usual commutation relations

$$[\hat{a}_j(T), \hat{a}_l(T)] = 0, \qquad \left[\hat{a}_3(T), \hat{a}_3^\dagger(T)\right] = \left[\hat{a}_4(T), \hat{a}_4^\dagger(T)\right] = 1, \qquad \left[\hat{a}_3(T), \hat{a}_4^\dagger(T)\right] = 0 \tag{6.87}$$

all hold.

The lossless assumption is an approximation because any optical component in practice is a little lossy, and S is not exactly unitary. The approximation may be acceptable, however, if the material of the beam splitter has very low loss (e.g., dielectrics, glasses, crystals) given the spectrum of the pulses, the bulk and the surfaces are very uniform so that there's little scattering into other modes, and your alignment of the optical beams is very good, etc.

There are also stringent requirements on the electric fields of the pulse modes so that the two input modes couple exactly into two output modes and not more. A detailed study of the requirements would require a deeper dive into classical optics that we won't attempt here; it suffices to say that the pulses should have **identical pulse shapes** (e.g., identical center frequency $\omega_0 = ck_0$, identical spectrum $g(\omega/c)$), their spectrum should fall on the transparent frequency band of the beam splitter where there is negligible loss and dispersion, and the pulses arrive at beam splitter at the right time, at the right spots, and at the correct angles. The timing issue is less of a problem if we have continuous-wave (CW) laser beams, which can be regarded as sequences of pulses.

At the end of the day, the main reason we make the assumption is simplicity: the input-output relation involves only two inputs and two outputs. We can worry about more complicated models later.

Exercise 6.10. Assume that V is unitary.

(1) Prove that Eq. (6.85) holds if and only if the scattering matrix S given by Eq. (6.84) is unitary.
(2) Prove that the scattering matrix S given by Eq. (6.84) is unitary if and only if

$$V_{j1}(T) = 0 \text{ and } V_{j2}(T) = 0 \text{ for } j \neq 3 \text{ and } j \neq 4. \tag{6.88}$$

(These exercises imply that, assuming that V is unitary, S is unitary if and only if V looks like this:

$$V = \begin{pmatrix} 0 & 0 & & & \\ 0 & 0 & & & \\ V_{31} & V_{32} & 0 & \dots & 0 \\ V_{41} & V_{42} & 0 & \dots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & & \\ 0 & 0 & & & \end{pmatrix}, \tag{6.89}$$

so $\hat{a}_3(T)$ and $\hat{a}_4(T)$ depend on $\hat{a}_1(0)$ and $\hat{a}_2(0)$ only ($V_{3j}(T) = V_{4j}(T) = 0$ for $j \neq 1$ and $j \neq 2$) and also no other output modes depend on $\hat{a}_1(0)$ and $\hat{a}_2(0)$ ($V_{j1}(T) = V_{j2}(T) = 0$ for $j \neq 3$ and $j \neq 4$.)

Exercise 6.11. Show that, given a unitary S, we have

$$|\alpha_3(T)|^2 + |\alpha_4(T)|^2 = |\alpha_1(0)|^2 + |\alpha_2(0)|^2 \tag{6.90}$$

in the classical case and

$$\hat{a}_3^\dagger(T)\hat{a}_3(T) + \hat{a}_4^\dagger(T)\hat{a}_4(T) = \hat{a}_1^\dagger(0)\hat{a}_1(0) + \hat{a}_2^\dagger(0)\hat{a}_2(0) \tag{6.91}$$

in the quantum case. Eq. (6.91) means that the total photon number is conserved (i.e., a measurement of the total output photon number at time t is equivalent to a measurement of the total input photon number at time 0).

(This is why we call a unitary S the lossless assumption.)

Exercise 6.12. A beam splitter is called **50-50** if

$$|\tau|^2 = |r|^2 = |\tau'|^2 = |r'|^2 = \frac{1}{2}, \tag{6.92}$$

since

$$|\alpha_3(T)|^2 = |\alpha_4(T)|^2 = \frac{1}{2}|\alpha_1(0)|^2 \tag{6.93}$$

if $\alpha_2(0)$ is zero and

$$|\alpha_3(T)|^2 = |\alpha_4(T)|^2 = \frac{1}{2}|\alpha_2(0)|^2 \tag{6.94}$$

if $\alpha_1(0)$ is zero. Find the relations among $\angle\tau$, $\angle r$, $\angle\tau'$, and $\angle r'$ if the scattering matrix is unitary.

Exercise 6.13. Prove that, if V is unitary and S is given by Eq. (6.84) in terms of $V_{31}, V_{32}, V_{41}, V_{42}$, then Eq. (6.82) implies

$$|\alpha_3(T)|^2 + |\alpha_4(T)|^2 \leq |\alpha_1(0)|^2 + |\alpha_2(0)|^2, \tag{6.95}$$

so the beam splitter is in general lossy in the context of classical optics.

Exercise 6.14. If the initial state for a lossless beam splitter is a coherent state for mode 1 and 2 and vacuum for all the other modes in a tensor product like this:

$$|\psi\rangle = |\alpha_1(0)\rangle \otimes |\alpha_2(0)\rangle \otimes |\text{vac}\rangle \otimes \cdots \otimes |\text{vac}\rangle\,. \tag{6.96}$$

What is the state at time T in the Schrödinger picture?

6.6.2. Schrödinger picture. Here we would like to derive something like Eq. (6.67) for a lossless beam splitter, which involves many modes in general, even though only four modes seem to matter in the Heisenberg picture.

From Exercise 6.9, we know that, for passive linear optics,

$$\hat{U}\hat{\rho}\hat{U}^\dagger = \int \Phi(V^\dagger\boldsymbol{\beta})\,|\boldsymbol{\beta}\rangle\,\langle\boldsymbol{\beta}|\,d^{2J}\boldsymbol{\beta}, \qquad (V^\dagger\boldsymbol{\beta})_j = \sum_k V_{kj}^*\beta_k, \tag{6.97}$$

where the T dependence of $\hat{U}(T)$ and $V(T)$ is not explicitly stated for brevity. From Exercise 6.10, we also know that, for a lossless beam splitter,

$$V_{k1} = V_{k2} = 0 \text{ for } k \neq 3 \text{ or } 4, \qquad V_{3j} = V_{4j} = 0 \text{ for } j \neq 1 \text{ or } 2. \tag{6.98}$$

Hence

$$\Phi(V^\dagger\boldsymbol{\beta}) = \Phi(V_{31}^*\beta_3 + V_{41}^*\beta_4, V_{32}^*\beta_3 + V_{42}^*\beta_4, \dots), \tag{6.99}$$

where the $\dots$ variables all do not depend on β_3 or β_4 and depend on $\beta_1, \beta_2, \beta_5, \beta_6, \dots$ only. Now if the initial state is separable like

$$\hat{\rho} = \hat{\rho}_{12} \otimes \hat{\rho}_{34\dots J}, \tag{6.100}$$

where $\hat{\rho}_{12}$ is the initial state for mode 1 and 2 and $\hat{\rho}_{34\dots J}$ is the initial state for the rest of the modes, we can write the initial $\Phi(\boldsymbol{\alpha})$ as

$$\Phi(\boldsymbol{\alpha}) = \Phi_{12}(\alpha_1, \alpha_2)\Phi_{34\dots J}(\alpha_3, \alpha_4, \dots), \tag{6.101}$$

where Φ_{12} is the Sudarshan representation of $\hat{\rho}_{12}$ and $\Phi_{34\dots}$ is that of $\hat{\rho}_{34\dots J}$. Then the Sudarshan representation of $\hat{U}\hat{\rho}\hat{U}^\dagger$ at time T becomes

$$\Phi(V^\dagger\boldsymbol{\beta}) = \Phi_{12}(V_{31}^*\beta_3 + V_{41}^*\beta_4, V_{32}^*\beta_3 + V_{42}^*\beta_4)\Phi_{34\dots J}(\dots). \tag{6.102}$$

This is separable as a product of $\Phi_{12}(V_{31}^*\beta_3 + V_{41}^*\beta_4, V_{32}^*\beta_3 + V_{42}^*\beta_4)$, which is a function of (β_3, β_4) only, and $\Phi_{34\dots J}(\dots)$, which does not depend on (β_3, β_4) and is a function of $\beta_1, \beta_2, \beta_5, \beta_6, \dots$ only. Hence

$$\begin{aligned}
&\hat{U}(\hat{\rho}_{12} \otimes \hat{\rho}_{34\dots J})\hat{U}^\dagger \\
&= \int \Phi_{12}(V_{31}^*\beta_3 + V_{41}^*\beta_4, V_{32}^*\beta_3 + V_{42}^*\beta_4)\Phi_{34\dots J}(\dots)\,|\beta_1, \beta_2, \dots\rangle\,\langle\beta_1, \beta_2, \dots|\,d^2\beta_1 d^2\beta_2 \dots d^2\beta_J \qquad (6.103)\\
&= \int \Phi_{34\dots J}(\dots)\,|\beta_1, \beta_2\rangle\,\langle\beta_1, \beta_2| \otimes \underbrace{\left[\int \Phi_{12}(V_{31}^*\beta_3 + V_{41}^*\beta_4, V_{32}^*\beta_3 + V_{42}^*\beta_4)\,|\beta_3, \beta_4\rangle\,\langle\beta_3, \beta_4|\,d^2\beta_3 d^2\beta_4\right]}_{\equiv\hat{\rho}_{34}(T)} \\
&\quad \otimes |\beta_5, \beta_6, \dots\rangle\,\langle\beta_5, \beta_6, \dots|\,d^2\beta_1 d^2\beta_2 d^2\beta_5 d^2\beta_6 \dots d^2\beta_J. \qquad (6.104)
\end{aligned}$$

This expression is a bit hard to read but it means that the state is separable as a tensor product of a density operator $\hat{\rho}_{34}(T)$ for mode 3,4 and a density operator for the other modes, as $\hat{\rho}_{34}(T)$ doesn't depend on $\beta_1, \beta_2, \beta_5, \beta_6, \dots$ and

is in some sense factorizable from the $\int(\dots)d^2\beta_1 d^2\beta_2 d^2\beta_5 d^2\beta_6\dots$ integral. In particular, if we take the partial trace with respect to mode 1,2,5,6,. . . , we obtain

$$\mathrm{tr}_{1256\dots}\left[\hat{U}(\hat{\rho}_{12}\otimes\hat{\rho}_{34\dots J})\hat{U}^\dagger\right]=\hat{\rho}_{34}(T). \tag{6.105}$$

This final state $\hat{\rho}_{34}(T)$ for mode 3 and 4 can be rewritten as

$$\hat{\rho}_{34}(T)=\int\Phi_{12}(V_{31}^*\beta_3+V_{41}^*\beta_4,V_{32}^*\beta_3+V_{42}^*\beta_4)\left|\beta_3,\beta_4\right\rangle\left\langle\beta_3,\beta_4\right|d^2\beta_3 d^2\beta_4 \tag{6.106}$$

$$=\int\Phi_{12}(\alpha_1,\alpha_2)\left|\begin{pmatrix}V_{31}&V_{32}\\V_{41}&V_{42}\end{pmatrix}\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}V_{31}&V_{32}\\V_{41}&V_{42}\end{pmatrix}\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right|d^2\alpha_1 d^2\alpha_2 \qquad \text{(change of variables)} \tag{6.107}$$

$$=\boxed{\int\Phi_{12}(\alpha_1,\alpha_2)\left|S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle\left\langle S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right|d^2\alpha_1 d^2\alpha_2,} \qquad \left(S=\begin{pmatrix}V_{31}&V_{32}\\V_{41}&V_{42}\end{pmatrix}\right) \tag{6.108}$$

where the change of variables is given by

$$\alpha_1=V_{31}^*\beta_3+V_{41}^*\beta_4,\qquad \alpha_2=V_{32}^*\beta_3+V_{42}^*\beta_4,\qquad \begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}=S^\dagger\begin{pmatrix}\beta_3\\\beta_4\end{pmatrix},\qquad \begin{pmatrix}\beta_3\\\beta_4\end{pmatrix}=S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}, \tag{6.109}$$

and we have written the coherent state for mode 3 and 4 as

$$\left|\beta_3,\beta_4\right\rangle=\left|\begin{pmatrix}\beta_3\\\beta_4\end{pmatrix}\right\rangle=\left|S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle. \tag{6.110}$$

Eq. (6.108) looks like Eq. (6.67), except that it involves the scattering matrix S of the beam splitter and the final state $\hat{\rho}_{34}(T)$ is for mode 3 and 4. For example, if the initial state for mode 1 and 2 is a coherent state

$$\hat{\rho}_{12}=\left|\alpha_1,\alpha_2\right\rangle\left\langle\alpha_1,\alpha_2\right|, \tag{6.111}$$

then

$$\Phi_{12}(\alpha_1',\alpha_2')=\delta^2(\alpha_1'-\alpha_1)\delta^2(\alpha_2'-\alpha_2),\quad \text{(changed dummy } (\alpha_1,\alpha_2) \text{ in Eq. (6.108) to } (\alpha_1',\alpha_2')) \tag{6.112}$$

$$\hat{\rho}_{34}(T)=\left|S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle\left\langle S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right|, \tag{6.113}$$

which is still a coherent state, and its amplitudes are given by the classical input-output relations for the beam splitter.

Exercise 6.15.

(1) Consider two modes 1 and 2 only. Show that a coherent state $\left|S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle_{12}$ for the two modes, where S is a unitary matrix, can be expressed as

$$\left|S\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle_{12}=\hat{U}\left|\begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}\right\rangle_{12},\qquad \hat{U}=\exp\left(-iT\sum_{j=1}^{2}\sum_{k=1}^{2}F_{jk}\hat{a}_j^\dagger\hat{a}_k\right),\qquad S=\exp(-iFT), \tag{6.114}$$

where $\hat{U}$ is a unitary operator.

(2) Define an operator $\hat{A}$ as

$$\hat{A}\equiv\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\left|n,m\right\rangle_{34}\left\langle n,m\right|_{12},\qquad \hat{A}\left|n,m\right\rangle_{12}=\left|n,m\right\rangle_{34}, \tag{6.115}$$

i.e., it maps any number state in $\mathcal{H}_1 \otimes \mathcal{H}_2$ to a number state in $\mathcal{H}_3 \otimes \mathcal{H}_4$ with the same numbers n, m. Show that it also maps any coherent state for mode 1 and 2 to a coherent state for mode 3 and 4 with the same amplitudes, i.e.,

$$\hat{A} \left|\beta_3, \beta_4\right\rangle_{12} = \left|\beta_3, \beta_4\right\rangle_{34}. \tag{6.116}$$

(3) Show that $\hat{A}$ is a unitary operator from $\mathcal{H}_1 \otimes \mathcal{H}_2$ to $\mathcal{H}_3 \otimes \mathcal{H}_4$, i.e., $\hat{A}^\dagger \hat{A} = \hat{I}_1 \otimes \hat{I}_2$ and $\hat{A}\hat{A}^\dagger = \hat{I}_3 \otimes \hat{I}_4$. Show that $\hat{A}\hat{U}$ is also a unitary operator from $\mathcal{H}_1 \otimes \mathcal{H}_2$ to $\mathcal{H}_3 \otimes \mathcal{H}_4$.

(4) For a lossless beamsplitter, show that we can write

$$\hat{\rho}_{34}(T) = \hat{B}\hat{\rho}_{12}\hat{B}^\dagger, \tag{6.117}$$

where $\hat{B} = \hat{A}\hat{U}$ is a unitary operator from $\mathcal{H}_1 \otimes \mathcal{H}_2$ to $\mathcal{H}_3 \otimes \mathcal{H}_4$, so that $\hat{\rho}_{34}(T)$ for mode 3 and 4 is related to the initial $\hat{\rho}_{12}$ for mode 1 and 2 through some unitary operator $\hat{B}$.

(Our construction of the unitary operator $\hat{B} = \hat{A}\hat{U}$ is mathematical, aiming to show that a unitary $\hat{B}$ exists mathematically to relate any input state to the output state for a beamsplitter with any unitary scattering matrix S. Deriving $\hat{B}$ from real physics would be much harder.)

CHAPTER 7

Loss

7.1. Heisenberg picture

The standard way of modeling optical loss in a material is to assume passive linear optics, where some of the modes are **inaccessible** to our experimenter. Those inaccessible modes can be matter modes, such as energy excitations in electrons or vibrations of the crystal, or EM modes, such as scattered light in directions we can't collect. For simplicity, let's consider loss in one optical mode, e.g., one pulse in an optical fiber. Let $\hat{a}_1(0)$ be the annihilation operator for a pulse mode at the input end of the fiber and $\hat{a}_3(T)$ be the operator for a pulse mode at the output end. If we peek at the classical equation

$$\alpha_3(T) = \tau\alpha_1(0), \tag{7.1}$$

where τ is the transmission coefficient with $|\tau|^2 < 1$, and just mindlessly write

$$\hat{a}_3(T) = \tau\hat{a}_1(0), \tag{7.2}$$

then

$$[\hat{a}_3(T), \hat{a}_3^\dagger(T)] = |\tau|^2[\hat{a}_1(0), \hat{a}_1^\dagger(0)] = |\tau|^2 < 1, \tag{7.3}$$

and we would have committed a cardinal sin in quantum mechanics: violating the commutation relation for an annihilation operator. Recall that $[\hat{a}_3(T), \hat{a}_3^\dagger(T)] = 1$ must hold for any t in the Heisenberg picture $\hat{a}_3(T) = \hat{U}^\dagger\hat{a}_3\hat{U}$ for any unitary $\hat{U}$; if $\hat{U}$ is not unitary, all hell breaks loose in quantum mechanics (e.g., probability is not conserved, Heisenberg uncertainty relations no longer hold.)

We are not so brave to break quantum mechanics in this book, so we correct our model. The minimal model that works is the two-input-two-output relation given by Eq. (6.86), just like that for a beam splitter, with a unitary S, as illustrated in Fig. 7.1. Now we have

$$\boxed{\hat{a}_3(T) = \tau\hat{a}_1(0) + r\hat{a}_2(0),} \tag{7.4}$$

including $\hat{a}_2(0)$ for an inaccessible input mode. Since S is unitary, $SS^\dagger = I$, meaning that

$$SS^\dagger = \begin{pmatrix} \tau & r \\ r' & \tau' \end{pmatrix}\begin{pmatrix} \tau^* & r'^* \\ r^* & \tau'^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{7.5}$$

In particular,

$$\boxed{|\tau|^2 + |r|^2 = 1.} \tag{7.6}$$

Most importantly, this relation allows $|\tau|^2$ to go below 1, so we can use it to model loss. With $[\hat{a}_j(0), \hat{a}_l^\dagger(0)] = \delta_{jl}$ for the two input modes, we obtain

$$[\hat{a}_3(T), \hat{a}_3^\dagger(T)] = |\tau|^2 + |r|^2 = 1, \tag{7.7}$$

which restores the fundamental commutation relation.

Side note. *$|\tau|^2$ must remain below 1 in this model. If you want to model an amplifier by making $|\tau|^2 > 1$, you'll have to go beyond passive linear optics (another topic for another day).*

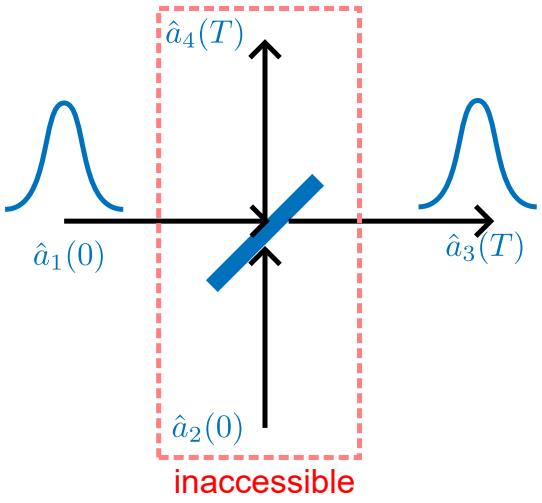

FIGURE 7.1. A beam-splitter model for optical loss.

Eq. (7.4) is the simplest example of a **quantum dissipation-fluctuation relation**: it says that, if there is dissipation (i.e., loss, with $|\tau|^2 < 1$), we need to include an additional input $\hat{a}_2(0)$, the mode of which is inaccessible and acts like a noise source.

Our output now depends on the initial state of the two input modes 1 and 2. Remember that mode 1 is something we can control, and mode 2 is inaccessible. A common assumption of the initial state is that mode 1 and 2 are initially independent, i.e., the density operator is given by

$$\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2, \tag{7.8}$$

and $\hat{\rho}_2$ is a thermal state. The output mean amplitude becomes

$$\mathrm{tr}\left[\hat{a}_3(T)\hat{\rho}\right] = \tau\,\mathrm{tr}\left[\hat{a}_1(0)\hat{\rho}_1\right] + r\,\mathrm{tr}\left[\hat{a}_2(0)\hat{\rho}_2\right]. \tag{7.9}$$

We obtain the classical Eq. (7.1) if $\mathrm{tr}[\hat{a}_2(0)\hat{\rho}_2] = 0$, which is indeed the case for a thermal $\hat{\rho}_2$.

More interestingly, suppose we measure the quadrature

$$\hat{q}_3(T) \equiv \frac{1}{\sqrt{2}}\left[\hat{a}_3(T) + \hat{a}_3^\dagger(T)\right] \tag{7.10}$$

$$= \frac{1}{\sqrt{2}}\left[\tau\hat{a}_1(0) + \tau^*\hat{a}_1^\dagger(0)\right] + \frac{1}{\sqrt{2}}\left[r\hat{a}_2(0) + r^*\hat{a}_2^\dagger(0)\right]. \tag{7.11}$$

then it can be shown that the variance is

$$\boxed{\left\langle \Delta q_3^2(T)\right\rangle = |\tau|^2\left\langle \Delta O_1^2(0)\right\rangle + |r|^2\left\langle \Delta O_2^2(0)\right\rangle,} \tag{7.12}$$

$$\hat{O}_1(0) \equiv \frac{1}{\sqrt{2}|\tau|}\left[\tau\hat{a}_1(0) + \tau^*\hat{a}_1^\dagger(0)\right], \tag{7.13}$$

$$\hat{O}_2(0) \equiv \frac{1}{\sqrt{2}|r|}\left[r\hat{a}_2(0) + r^*\hat{a}_2^\dagger(0)\right]. \tag{7.14}$$

where $\hat{O}_1(0)$ and $\hat{O}_2(0)$ are quadrature operators of mode 1 and 2, $\left\langle \Delta O_1^2(0)\right\rangle$ is in terms of $\hat{\rho}_1$, and $\left\langle \Delta O_2^2(0)\right\rangle$ is in terms of $\hat{\rho}_2$. We see that, in the quantum case, an additional variance $\left\langle \Delta O_2^2(0)\right\rangle$ due to mode 2 must contribute to the output variance—this is why I said earlier that mode 2 acts like a noise source and why we call Eq. (7.4) a dissipation-fluctuation relation. For a thermal $\hat{\rho}_2$ with mean number $\langle n_2\rangle$ in particular,

$$\left\langle \Delta O_2^2(0)\right\rangle = \langle n_2\rangle + \frac{1}{2}. \tag{7.15}$$

Even if $\hat{\rho}_2$ is vacuum ($\langle n_2\rangle = 0$), this term is still nonzero.

Exercise 7.1. Verify Eq. (7.12).

Exercise 7.2. An optical pulse passes through two lossy optical components. For the first component, the input-output relation is

$$\hat{a}_3(T) = \tau_1 \hat{a}_1(0) + r_1 \hat{a}_2(0), \qquad |\tau_1|^2 + |r_1|^2 = 1, \tag{7.16}$$

and for the second component, the input-output relation is

$$\hat{a}_5(T+T') = \tau_2 \hat{a}_3(T) + r_2 \hat{a}_6(0), \qquad |\tau_2|^2 + |r_2|^2 = 1, \tag{7.17}$$

where mode 6 is another inaccessible mode. Show that the net input-output relation can be expressed as

$$\hat{a}_5(T+T') = \tau \hat{a}_1(0) + r\hat{b}(0), \tag{7.18}$$

where τ and r also satisfy Eq. (7.6) and $\hat{b}(0)$ is the annihilation operator for a new mode in terms of $\hat{a}_2(0)$ and $\hat{a}_6(0)$.

(The point of this exercise is to show that Eqs. (7.4) and (7.6) can model cascaded losses, so they are quite general.)

Exercise 7.3. Suppose that $\hat{\rho}_1 = |\alpha\rangle\langle\alpha|$ is a coherent state and $\hat{\rho}_2$ is vacuum.

(1) Find $\langle \Delta q_3^2(T) \rangle$.

(2) The signal-to-noise ratio (SNR) of the measurement is defined as

$$\text{SNR} \equiv \frac{\langle q_3(T)\rangle^2}{\langle \Delta q_3^2(T)\rangle}, \tag{7.19}$$

$$\langle q_3(T)\rangle \equiv \text{tr}\,[\hat{q}_3(T)\hat{\rho}_1]. \tag{7.20}$$

Find the SNR in terms of

$$\langle O_1(0)\rangle \equiv \text{tr}[\hat{O}_1(0)\hat{\rho}_1] \tag{7.21}$$

and call it $\text{SNR}_{|\alpha\rangle}$.

(3) Suppose now that $\hat{\rho}_1$ is a "squeezed" state with the same initial mean $\langle O_1(0)\rangle$ as that of the coherent state, but its initial variance of $\hat{O}_1$ is given by

$$\langle \Delta O_1^2(0)\rangle = \frac{s}{2}, \tag{7.22}$$

where $s \leq 1$ is a squeezing parameter. Find the SNR when $|\tau|^2 = 1$. Find $\text{SNR}/\text{SNR}_{|\alpha\rangle}$, i.e., how much the SNR is enhanced relative to a coherent state when there is no loss. Find $\text{SNR}/\text{SNR}_{|\alpha\rangle}$ for a given $|\tau|^2$ and s.

(4) Assume a fixed $s < 1$. If $|\tau|^2$ is reduced, does $\text{SNR}/\text{SNR}_{|\alpha\rangle}$ increase or decrease? What is $\text{SNR}/\text{SNR}_{|\alpha\rangle}$ as $|\tau|^2 \to 0$?

(5) If $s = 0.1$, plot $\text{SNR}/\text{SNR}_{|\alpha\rangle}$ as a function of $0 \leq |\tau|^2 \leq 1$. Find the minimum $|\tau|^2$ so that $\text{SNR}/\text{SNR}_{|\alpha\rangle} \geq 2$, i.e., find the minimum transmission so that there remains a 3dB enhancement.

(This exercise shows how loss affects the SNR in a simple sensing problem.)

7.2. Schrödinger picture

The way we model loss by passive linear optics is an example of a more general strategy of modeling an **open quantum system** that interacts with an environment.

(1) At $t = 0$, there are some **accessible** degrees of freedom that we call **system A** and some **inaccessible** degrees of freedom that we call **system B** or the initial bath. Let $\hat{\rho}_A$ be the density operator of system A and $\hat{\rho}_B$ be that of system B.
- In the beam-splitter model of loss, system A would be the input mode 1 and system B would be the input mode 2 (and everything else).

(2) Over time, system A and B may interact. The dynamics is modeled by a unitary operator $\hat{U}$.

(3) At final time T, again only some degrees of freedom are accessible and some are not. We call the accessible part at time T **system C**, which may not be the same as system A. We call the inaccessible part at time T **system D** or the final bath.
   - In the beam-splitter model, system C would be the output mode 3. System D would be the output mode 4 and everything else.

The Schrödinger picture is more popular in open quantum system theory, and the main problem in the Schrödinger picture is to compute the density operator of the accessible system C at time T, which is given by

$$\boxed{\hat{\rho}_C(T) = \mathrm{tr}_D\left[\hat{U}(\hat{\rho}_A \otimes \hat{\rho}_B)\hat{U}^\dagger\right],} \tag{7.23}$$

where tr_D is the **partial trace** over the inaccessible system-D Hilbert space (see Sec. B.10.2). **Decoherence** of a system, in particular, is modeled this way. Once we have $\hat{\rho}_C(T)$, we can compute the probability distribution of any measurement on system C at time T using Born's rule.

Eq. (7.23) is usually difficult to solve, but we can use Sec. 6.6.2, and Eq. (6.108) in particular, for our beam-splitter model of loss. At $t = 0$, $\hat{\rho}_A = \hat{\rho}_1$ is the state of the first input mode, and $\hat{\rho}_B = \hat{\rho}_2 \otimes \hat{\rho}_{34\ldots J}$ is the state of the initial bath. After the beam-splitter interaction, Eq. (6.108) gives the density operator $\hat{\rho}_{34}(T)$ for output mode 3 (system C) and output mode 4 (part of system D). We can compute $\hat{\rho}_C(T) = \hat{\rho}_3(T)$ from $\hat{\rho}_{34}(T)$ simply by tracing out mode 4:

$$\hat{\rho}_3(T) = \mathrm{tr}_4\left[\hat{\rho}_{34}(T)\right] = \mathrm{tr}_4 \int \Phi_{12}(\alpha_1,\alpha_2) \left|S\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}\right\rangle \left\langle S\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}\right| d^2\alpha_1 d^2\alpha_2 \tag{7.24}$$

$$= \int \Phi_{12}(\alpha_1,\alpha_2)\, \mathrm{tr}_4 \left[\left|S\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}\right\rangle \left\langle S\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}\right|\right] d^2\alpha_1 d^2\alpha_2. \tag{7.25}$$

$\Phi_{12}(\alpha_1,\alpha_2)$, the Sudarshan representation of mode 1 and 2, is the product of the representation $\Phi_1(\alpha_1)$ for mode 1 and $\Phi_2(\alpha_2) = \delta^2(\alpha_2)$ for mode 2, assumed to be in vacuum state here. The partial trace of a coherent state is also easy, since the coherent state is separable. Let

$$\begin{pmatrix}\beta_3\\ \beta_4\end{pmatrix} = S\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \begin{pmatrix}\tau\alpha_1 + r\alpha_2\\ r'\alpha_1 + \tau'\alpha_2\end{pmatrix}. \tag{7.26}$$

Then the partial trace is simply

$$\mathrm{tr}_4\left(|\beta_3,\beta_4\rangle\langle\beta_3,\beta_4|\right) = \mathrm{tr}_4\left(|\beta_3\rangle\langle\beta_3| \otimes |\beta_4\rangle\langle\beta_4|\right) = \mathrm{tr}_4\left(|\beta_3\rangle\langle\beta_3| \otimes |\beta_4\rangle\langle\beta_4|\right) = |\beta_3\rangle\langle\beta_3|, \tag{7.27}$$

where $\beta_3 = \tau\alpha_1 + r\alpha_2$. Hence

$$\hat{\rho}_3(T) = \int \Phi_1(\alpha_1)\delta^2(\alpha_2)\,|\tau\alpha_1 + r\alpha_2\rangle\langle\tau\alpha_1 + r\alpha_2|\, d^2\alpha_1 d^2\alpha_2 = \boxed{\int \Phi_1(\alpha_1)\,|\tau\alpha_1\rangle\langle\tau\alpha_1|\, d^2\alpha_1.} \tag{7.28}$$

For example, if the input mode 1 is in a coherent state,

$$\hat{\rho}_1 = |\alpha\rangle\langle\alpha|, \qquad \Phi_1(\alpha_1) = \delta^2(\alpha_1 - \alpha), \tag{7.29}$$

then the state of output mode 3 is simply the coherent state

$$\boxed{\hat{\rho}_3(T) = |\tau\alpha\rangle\langle\tau\alpha|} \tag{7.30}$$

with a reduced amplitude.

We can draw two conclusions from this calculation:

(1) A classical state with a nonnegative Sudarshan representation $\Phi_1(\alpha_1)$ will remain a classical state after loss, since $\hat{\rho}_3(T)$ also has a nonnegative Sudarshan representation (Exercise 7.4).
(2) A coherent state will remain a coherent state after loss, even though the amplitude is reduced.

A nonclassical input state, on the other hand, is less robust to loss and become less nonclassical, but it is outside the scope of this course to study what happens there; you may go through Exercise 7.5 to get a taste of what's going on.

Exercise 7.4. Find the Sudarshan representation $\Phi_3(\alpha_3, T)$ of $\hat{\rho}_3(T)$ from Eq. (7.28). Show that, if $\Phi_1(\alpha_1) \geq 0$ for all α_1, then $\Phi_3(\alpha_3, T)$ also stays nonnegative for all α_3.

Exercise 7.5. (Numerical exercise). Assume that there are only two modes 1 and 2 for simplicity and a unitary operator given by

$$\hat{U}(T) = \exp\left(-iT \sum_{j=1}^{2} \sum_{k=1}^{2} F_{jk} \hat{a}_j^\dagger \hat{a}_k\right). \tag{7.31}$$

(1) If the Heisenberg equations of motion are given by

$$\hat{a}_1(T) = \tau \hat{a}_1(0) + r\hat{a}_2(0), \qquad \hat{a}_2(T) = r'\hat{a}_1(0) + \tau'\hat{a}_2(0), \tag{7.32}$$

find FT in terms of $S = \begin{pmatrix} \tau & r \\ r' & \tau' \end{pmatrix}$.

(2) Assume initial states $\hat{\rho}_1 = |n_1\rangle \langle n_1|$ and $\hat{\rho}_2 = |0\rangle \langle 0|$. Compute the final density matrix $\langle n| \hat{\rho}_1(T) |m\rangle$ of mode 1 in the Schrödinger picture

$$\hat{\rho}_1(T) = \mathrm{tr}_2 \left[\hat{U}(\hat{\rho}_1 \otimes \hat{\rho}_2)\hat{U}^\dagger\right]. \tag{7.33}$$

(3) Compute the entropy of the state given by

$$S \equiv -\,\mathrm{tr}\,[\hat{\rho}_1(T) \ln \hat{\rho}_1(T)], \tag{7.34}$$

for various values of n_1 and $|\tau|^2$. The operator logarithm $\ln \hat{\rho}_1(T)$ can be computed by the matrix logarithm https://en.wikipedia.org/wiki/Logarithm_of_a_matrix. Observe how the entropy changes as a function of n_1 and $|\tau|^2$.

CHAPTER 8

Measurements

8.1. Simple and generalized measurements

The simplest kind of quantum measurement can be modeled by assuming an orthonormal basis of the Hilbert space $\{|e_n\rangle : n = 1, 2, \dots\}$, such that the probability of an outcome $n \in \{1, 2, \dots\}$ is given by

$$P_n = \langle e_n| \hat{\rho} |e_n\rangle . \tag{8.1}$$

The jargons "von Neumann measurements" and "projective measurements" in the literature are all essentially this simple kind. We've already encountered some examples in quantum optics, such as photon counting. If the outcome is a continuous variable, we use Dirac's trick to write down a probability density, as reviewed in Appendix D.

The most general model of quantum measurement assumes that we can enlist an **ancilla** system for help (ancilla is a fancy word for an aid). The density operator of the system augmented by the ancilla would be $\hat{\rho} \otimes \hat{\rho}_B$, and then we model the measurement on the augmented system using an orthonormal basis $\{|f_n\rangle\}$ on the larger Hilbert space:

$$P_n = \langle f_n| \hat{\rho} \otimes \hat{\rho}_B |f_n\rangle . \tag{8.2}$$

All quantum measurements can be modeled this way.

The variety of quantum measurements allowed by these rules is huge in theory, but in practice we can only perform some of them in optics. This chapter discusses some basic types of measurements in quantum optics and how they can be implemented experimentally.

The discussion will be simple and idealistic, even though real devices will have all sorts of technical imperfections. To model those technical imperfections mathematically, we would have to use a lot more probability theory, so we won't go there.

8.2. Photon counting

We use the usual number basis to model ideal photon counting. For one mode, the outcome would have a probability distribution given by

$$P_n = \langle n| \hat{\rho} |n\rangle . \tag{8.3}$$

For J modes, the probability distribution is now a function of J photon numbers:

$$P_{n_1,\dots,n_J} = \langle n_1, \dots, n_J| \hat{\rho} |n_1, \dots, n_J\rangle . \tag{8.4}$$

These are ideal assumptions. In current technology, even the best photodetectors, e.g., avalanche photodiodes and transition-edge detectors, have a lot of technical problems, such as

(1) Poor photon-number resolution: they can't tell exactly the number of photons, e.g., they can only tell if it's zero or nonzero, or they can give only a rough range of the photon numbers, not the precise number.
(2) Inefficiency: only a fraction of the photons can be detected.
(3) Dark counts: Even when there is no photon, there are false-positive counts.
(4) Thermal noise: the electronics in the detector may add thermal noise to the signal. Similar to dark counts. This is why a lot of photodetectors need to be cooled for optimal performance.
(5) Dead time: After a detection event, certain detectors would take some time to reset before it can detect photons again.

Because of these problems, one needs to make a lot of measurements and do a lot of calibration and data processing in quantum optics experiments, or buy very expensive detectors that have better specs. If the detector is bad, experimental results can still be consistent with quantum calculations for the expected values, such as $\mathrm{tr}(\hat{n}\hat{\rho})$, since one can take many measurements and compute the sample average to reduce the noise, but we shouldn't expect the variance of the experimental outcome or the probability distribution to agree well with Born's rule, unless the experiment is amazingly good.

Technical problems notwithstanding, all photodetectors at optical frequencies (infrared, visible, etc.) perform some version of photon counting, i.e., they measure the optical energy or power. Since energy and power are the square of the EM fields, they are also called **square-law detectors**.

Side note. *Sometimes people reserve the name "photon counting" for detectors that can have very good photon-number resolution, but let's not be pedantic here.*

8.3. Homodyne detection

Since we only have square-law detectors in optics, we'd need a more complicated setup if we want to measure other observables, e.g., the quadratures. A standard approach to measure a quadrature is homodyne detection: Combine an optical beam with another much stronger beam called the **local oscillator**, typically a laser beam, using a beam splitter, and then measure the photon numbers of the two output ports, as depicted in Fig. 8.1.

Side note. *"Homo" in the word homodyne means "same" and refers to the fact that, in the limit of infinitely long pulses (called continuous wave or CW in optics), the local oscillator and the signal have the same frequency $\omega_0 = ck_0$. For the pulses considered here, their electric fields need to match very well for the two-input-two-output relation to hold, as discussed earlier, not just the center frequency. "Dyne" means "power" in Greek; presumably it refers to the local oscillator.*

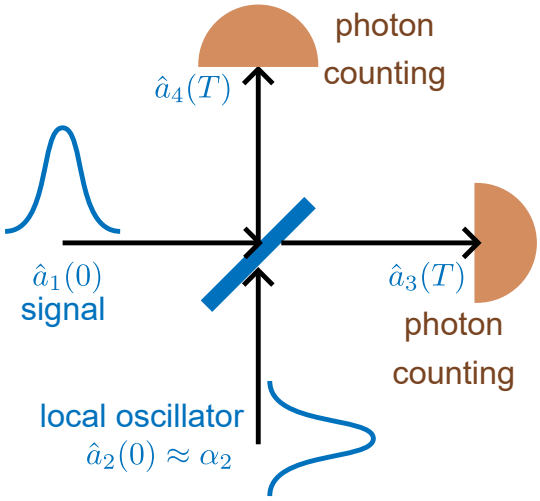

FIGURE 8.1. Homodyne detection using a 50-50 beam splitter, a local oscillator, and photon counting in the two output modes.

For simplicity, we follow Sec. 6.6 and assume for now that there is just one optical pulse we'd like to measure, called the signal. Let input 1 be the signal pulse and input 2 be the strong local oscillator. We also assume that the beam splitter is lossless and **50-50**, i.e.,

$$|\tau|^2 = |r|^2 = |\tau'|^2 = |r'|^2 = \frac{1}{2}. \tag{8.5}$$

Since the scattering matrix is unitary, $SS^\dagger = S^\dagger S = I$, we also have

$$\tau^* r' + r^* \tau' = 0, \qquad \tau^* r + r'^* \tau' = 0. \tag{8.6}$$

In the Heisenberg picture, the output photon numbers for the output pulse modes become (omitting the dependence of the operators on time for brevity)

$$\hat{a}_3^\dagger \hat{a}_3 = \Big(\tau^* \hat{a}_1^\dagger + r^* \hat{a}_2^\dagger\Big)(\tau \hat{a}_1 + r \hat{a}_2) = |\tau|^2 \hat{a}_1^\dagger \hat{a}_1 + \tau^* r \hat{a}_1^\dagger \hat{a}_2 + \tau r^* \hat{a}_1 \hat{a}_2^\dagger + |r|^2 \hat{a}_2^\dagger \hat{a}_2, \tag{8.7}$$

$$\hat{a}_4^\dagger \hat{a}_4 = \Big(r'^* \hat{a}_1^\dagger + \tau'^* \hat{a}_2^\dagger\Big)\big(r' \hat{a}_1 + \tau' \hat{a}_2\big) = |r'|^2 \hat{a}_1^\dagger \hat{a}_1 + r'^* \tau' \hat{a}_1^\dagger \hat{a}_2 + r' \tau'^* \hat{a}_1 \hat{a}_2^\dagger + |\tau'|^2 \hat{a}_2^\dagger \hat{a}_2. \tag{8.8}$$

For a 50-50 beam splitter, these can be rewritten as

$$\hat{a}_3^\dagger \hat{a}_3 = \frac{1}{2}\Big(\hat{a}_1^\dagger \hat{a}_1 + e^{i\theta} \hat{a}_1^\dagger \hat{a}_2 + e^{-i\theta} \hat{a}_1 \hat{a}_2^\dagger + \hat{a}_2^\dagger \hat{a}_2\Big), \tag{8.9}$$

$$\hat{a}_4^\dagger \hat{a}_4 = \frac{1}{2}\Big(\hat{a}_1^\dagger \hat{a}_1 - e^{i\theta} \hat{a}_1^\dagger \hat{a}_2 - e^{-i\theta} \hat{a}_1 \hat{a}_2^\dagger + \hat{a}_2^\dagger \hat{a}_2\Big), \tag{8.10}$$

where

$$\theta \equiv \angle(\tau^* r) \tag{8.11}$$

is the phase of the complex number $\tau^* r$. Now let's focus on the observable

$$\hat{O} \equiv \hat{a}_3^\dagger \hat{a}_3 - \hat{a}_4^\dagger \hat{a}_4 = e^{i\theta} \hat{a}_1^\dagger \hat{a}_2 + e^{-i\theta} \hat{a}_1 \hat{a}_2^\dagger, \tag{8.12}$$

which can be measured by measuring the two output photon numbers and then subtract one from the other. When the local oscillator is much stronger than the signal, we can model it as classical. In quantum mechanics, we model a classical degree of freedom by replacing its operators by their means as classical numbers. Here we replace $\hat{a}_2$ by the complex amplitude α_2 of the local-oscillator pulse. Then

$$\boxed{\hat{O} \approx e^{-i\theta} \alpha_2^* \hat{a}_1 + e^{i\theta} \alpha_2 \hat{a}_1^\dagger.} \tag{8.13}$$

This is now a **quadrature** operator (see Exercise 4.26), i.e., a Hermitian linear combination of $\hat{a}_1$ and $\hat{a}_1^\dagger$. We can write

$$\hat{O} = |\alpha_2|\Big(e^{-i\theta - i\angle\alpha_2} \hat{a}_1 + \text{H.c.}\Big), \tag{8.14}$$

which shows that, by changing the phase $\angle\alpha_2$ of the local-oscillator amplitude α_2, one can measure a different quadrature. For example, if we set

$$\angle\alpha_2 = -\theta, \tag{8.15}$$

then

$$\hat{O} = |\alpha_2|\Big(\hat{a}_1 + \hat{a}_1^\dagger\Big), \tag{8.16}$$

which is proportional to the q-quadrature operator $\hat{q}_1 \equiv (\hat{a}_1 + \hat{a}_1^\dagger)/\sqrt{2}$. If we set

$$\angle\alpha_2 = -\theta + \frac{\pi}{2}, \tag{8.17}$$

then

$$\hat{O} = \frac{|\alpha_2|}{i}\Big(\hat{a}_1 - \hat{a}_1^\dagger\Big), \tag{8.18}$$

which is proportional to the p-quadrature operator $\hat{p}_1 \equiv (\hat{a}_1 - \hat{a}_1^\dagger)/(\sqrt{2}i)$. With a measurement of $\hat{O}$, we can just divide the outcome by some constant and it'd be equivalent to the usual measurement of a quadrature studied in Exercise 4.26.

It is remarkable that homodyne detection with photodiodes in practice can be quite close to ideal ($> 99\%$ efficiency, meaning that 99% of the noise variance comes from quantum) [9], unlike photon counting. It has something to do with the fact that photodiodes work much better at high optical energy, and photon-number resolution is not really required with homodyne.

Side note. *We have taken the classical approximation of the local oscillator as given and replaced $\hat{a}_2$ with α_2 without justification, but its validity can be studied more carefully by assuming that the local oscillator is in a coherent state $|\alpha_2\rangle$, and then take the limit of $|\alpha_2| \to \infty$ [10, 11]. The probability distribution of the exact $\hat{O}$ given by Eq. (8.12) can be shown to approach that of the approximate $\hat{O}$ given by Eq. (8.13). Exercise 8.2 asks you to check this approximation for the mean and the variance.*

Exercise 8.1. Suppose that the q-quadrature operator $\hat{q}_1 \equiv (\hat{a}_1 + \hat{a}_1^\dagger)/\sqrt{2}$ has the diagonal form

$$\hat{q}_1 = \int_{-\infty}^{\infty} x \, |q_1 = x\rangle \langle q_1 = x| \, dx, \tag{8.19}$$

where $\hat{q}_1 |q_1 = x\rangle = x |q_1 = x\rangle$ and $\langle q_1 = x | q_1 = x'\rangle = \delta(x - x')$. Let the diagonal form of the $\hat{O}$ given by Eq. (8.16) be

$$\hat{O} = \int_{-\infty}^{\infty} \lambda \, |O = \lambda\rangle \langle O = \lambda| \, d\lambda, \tag{8.20}$$

where $\hat{O} |O = \lambda\rangle = \lambda |O = \lambda\rangle$ and $\langle O = \lambda | O = \lambda'\rangle = \delta(\lambda - \lambda')$.

(1) Find $|O = \lambda\rangle$ in terms of $|q_1 = x\rangle$.
(2) Find the probability density of $\hat{O}$ if the state is
   (a) a number state $|n\rangle$,
   (b) a coherent state $|\alpha\rangle$.

Exercise 8.2. Let the exact $\hat{O}$ given by Eq. (8.12) be $\hat{O}$ and the approximation given by Eq. (8.13) be $\hat{O}'$. Let the second input mode be a coherent state $|\alpha_2\rangle$, so that the total state for the two input modes is $|\psi\rangle \otimes |\alpha_2\rangle$.

(1) Show that the means $\langle O\rangle$ and $\langle O'\rangle$ are equal.
(2) Show that the variances are related by

$$\langle \Delta O^2 \rangle = \langle \Delta O'^2 \rangle + \langle \psi | \, \hat{a}_1^\dagger \hat{a}_1 \, |\psi\rangle \, . \tag{8.21}$$

(3) If the first input is a coherent state $|\psi\rangle = |\alpha\rangle$, show that the difference between the two variances in part (2) is negligible if

$$|\alpha_2|^2 \gg |\alpha|^2. \tag{8.22}$$

8.4. Dual-homodyne detection

What if we want to measure both quadratures of the same pulse mode? One way is to use a beam splitter to split the signal beam into two, and then measure the two quadratures of the two outputs using two homodyne setups discussed in Sec. 8.3, as illustrated in Fig. 8.2.

To compute the probability density of this dual-homodyne setup, we again have to bear in mind that there are always two inputs and two outputs for a beam splitter in the quantum case. Assume that the second input is in a vacuum state $|0\rangle$. Let's study what happens when the signal is in a coherent state $|\alpha\rangle$ first, and then use the Sudarshan trick to generalize the result.

With mode 1 in a coherent state $|\alpha\rangle$ and mode 2 in vacuum $|0\rangle$, the multimode state $|\alpha\rangle_1 \otimes |0\rangle_2$ is also a coherent state. For simplicity, we'll assume that the beam splitter has the scattering matrix

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{8.23}$$

so it's lossless and 50-50. At the output, the state in the Schrödinger picture is also a coherent state, but now the amplitudes for mode 3 and 4 become $\alpha/\sqrt{2}$ and $\alpha/\sqrt{2}$, respectively, i.e., the output state for mode 3 and 4 can be expressed as

$$\left|\alpha/\sqrt{2}\right\rangle_3 \otimes \left|\alpha/\sqrt{2}\right\rangle_4 . \tag{8.24}$$

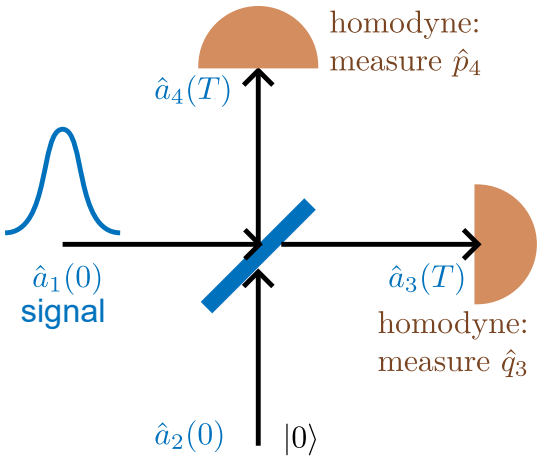

FIGURE 8.2. Dual-homodyne detection.

Then we perform measurements of $\hat{q}_3 \equiv (\hat{a}_3 + \hat{a}_3^\dagger)/\sqrt{2}$ and $\hat{p}_4 \equiv (\hat{a}_4 - \hat{a}_4^\dagger)/(\sqrt{2}i)$ via two homodyne detectors. The probability density becomes

$$f(x,y|\alpha) = \left|(\langle q_3 = x| \otimes \langle p_4 = y|)\left(\left|\alpha/\sqrt{2}\right\rangle_3 \otimes \left|\alpha/\sqrt{2}\right\rangle_4\right)\right|^2 \tag{8.25}$$

$$= \frac{1}{\pi}\exp\left[-(x - \operatorname{Re}\alpha)^2 - (y - \operatorname{Im}\alpha)^2\right], \tag{8.26}$$

where I've used Eqs. (4.7) and (4.8) back in Chapter 4 and I've inserted the symbol α into $f(x,y|\alpha)$ to emphasize that the probability density is conditioned on the amplitude α of the coherent state.

There is actually a more elegant expression of this probability density. Recall that two coherent states $|\alpha\rangle$ and $\langle\beta|$ have the inner product

$$|\langle\beta|\alpha\rangle|^2 = \exp\left(-|\beta - \alpha|^2\right) = \exp\left[-(\operatorname{Re}\beta - \operatorname{Re}\alpha)^2 - (\operatorname{Im}\beta - \operatorname{Im}\alpha)^2\right]. \tag{8.27}$$

This looks like Eq. (8.26) if we take

$$\boxed{\beta = x + iy.} \tag{8.28}$$

Then Eq. (8.26) can be rewritten in terms of the complex β as

$$\boxed{f(x,y|\alpha) = f(\operatorname{Re}\beta, \operatorname{Im}\beta|\alpha) = \frac{1}{\pi}|\langle\beta|\alpha\rangle|^2 = \frac{1}{\pi}\langle\beta|\alpha\rangle\langle\alpha|\beta\rangle.} \tag{8.29}$$

In other words, instead of taking the two real numbers (x,y) as the outcomes of the dual-homodyne setup, we can equally well assume that the outcome is one complex number $\beta = x + iy$, and the probability density has a simple expression given by Eq. (8.29). It says that we can simply sandwich the density operator $|\alpha\rangle\langle\alpha|$ between the coherent-state bra $\langle\beta|$ and ket $|\beta\rangle$ and then divide the result by π.

Now if the initial state $\hat{\rho}$ of mode 1 is arbitrary, the probability density for dual-homodyne looks like

$$f(x,y) = \langle q_3 = x, p_4 = y|\,\hat{U}(\hat{\rho} \otimes |\text{vac}\rangle\langle\text{vac}|)\hat{U}^\dagger\,|q_3 = x, p_4 = y\rangle \tag{8.30}$$

where $|\text{vac}\rangle$ denotes that all the other modes are in vacuum state, $\hat{U}$ models the dynamics due to the beam splitter, and $|q_3 = x, p_4 = y\rangle$ models the homodyne measurements at the two outputs. The expression looks scary, but if we write $\hat{\rho}$ in terms of the Sudarshan representation $\hat{\rho} = \int \Phi(\alpha)\,|\alpha\rangle\langle\alpha|\,d^2\alpha$, then we obtain

$$f(x,y) = \int \Phi(\alpha)\underbrace{\langle q_3 = x, p_4 = y|\,\hat{U}(|\alpha\rangle\langle\alpha| \otimes |\text{vac}\rangle\langle\text{vac}|)\hat{U}^\dagger\,|q_3 = x, p_4 = y\rangle}_{f(x,y|\alpha)}\,d^2\alpha. \tag{8.31}$$

Lo and behold, the underbraced expression is simply the probability density $f(x,y|\alpha)$ for dual-homodyne given an initial coherent state $|\alpha\rangle\langle\alpha|$. Hence

$$f(x,y) = \int \Phi(\alpha) f(x,y|\alpha) d^2\alpha \tag{8.32}$$

$$= \frac{1}{\pi}\int \Phi(\alpha)\,\langle\beta|\alpha\rangle\,\langle\alpha|\beta\rangle\,d^2\alpha \qquad \text{(using Eq. (8.29))} \tag{8.33}$$

$$= \frac{1}{\pi}\langle\beta|\left[\int \Phi(\alpha)\,|\alpha\rangle\langle\alpha|\,d^2\alpha\right]|\beta\rangle = \boxed{\frac{1}{\pi}\langle\beta|\,\hat{\rho}\,|\beta\rangle\,.} \tag{8.34}$$

This is the general expression for the probability density for the dual-homodyne detection—simply sandwich $\hat{\rho}$ between the coherent-state bra $\langle\beta|$ and ket $|\beta\rangle$, and then divide by π. The outcome is a complex number β; one homodyne detector gives its real part, and the other homodyne detector gives its imaginary part.

Dual-homodyne detection is an example of generalized measurements. The ancilla in this case is the second input mode shown in Fig. 8.2. With this generalized measurement, we are able to measure both quadratures of an optical mode, which would not be possible with one simple homodyne measurement.

There is a price to pay with this generalized measurement, however. Imagine a communication scenario: the sender prepares a pulse in a coherent state $|\alpha\rangle$ with one complex parameter α. The receiver measures it by homodyne or dual-homodyne, and the receiver's goal is to estimate the unknown complex parameter α given its measurement outcomes. First, let's assume that the receiver uses simple homodyne to measure $\hat{q}$. Recall from Chapter 4 that a simple quadrature measurement has the statistics

$$\langle q\rangle = \sqrt{2}\,\mathrm{Re}\,\alpha, \qquad\qquad \langle\Delta q^2\rangle = \frac{1}{2}. \tag{8.35}$$

This homodyne detection is sensitive to $\mathrm{Re}\,\alpha$ only, not $\mathrm{Im}\,\alpha$, as the probability density doesn't depend on $\mathrm{Im}\,\alpha$ at all. The signal-to-noise ratio would be

$$\mathrm{SNR}(\hat{q}) \equiv \frac{\langle q\rangle^2}{\langle\Delta q^2\rangle} = 4(\mathrm{Re}\,\alpha)^2. \tag{8.36}$$

With homodyne, the receiver could also have chosen to measure another quadrature, say, $\hat{p}$, giving

$$\mathrm{SNR}(\hat{p}) \equiv \frac{\langle p\rangle^2}{\langle\Delta p^2\rangle} = 4(\mathrm{Im}\,\alpha)^2, \tag{8.37}$$

but the homodyne detector must pick one quadrature to measure, never both in one measurement.

Dual homodyne, on the other hand, is sensitive to both $\mathrm{Re}\,\alpha$ and $\mathrm{Im}\,\alpha$, since Eq. (8.26) implies that

$$\langle q_3\rangle = \mathrm{Re}\,\alpha, \qquad \langle p_4\rangle = \mathrm{Im}\,\alpha, \qquad \langle\Delta q_3^2\rangle = \langle\Delta p_4^2\rangle = \frac{1}{2}. \tag{8.38}$$

The variances remain the same, because the outputs 3 and 4 are still in a coherent state, but the means are reduced by a factor of $\sqrt{2}$, because of the beam splitter. The SNR's become

$$\mathrm{SNR}(\hat{q}_3) = \frac{\langle q_3\rangle^2}{\langle\Delta q_3^2\rangle} = 2(\mathrm{Re}\,\alpha)^2, \qquad\qquad \mathrm{SNR}(\hat{p}_4) = \frac{\langle p_4\rangle^2}{\langle\Delta p_4^2\rangle} = 2(\mathrm{Im}\,\alpha)^2, \tag{8.39}$$

each of which is a factor of 2 lower than that of a simple homodyne measurement. This reduction in the SNR's is the penalty we have to pay for measuring both quadratures in one generalized measurement.

Exercise 8.3. Prove that $\iint \frac{1}{\pi}\langle\beta|\,\hat{\rho}\,|\beta\rangle\,d^2\beta = 1$, i.e., the probability density is normalized.

Exercise 8.4. Compute the probability density of the outcome from dual-homodyne detection if

(1) $\hat{\rho}$ is a coherent state $|\alpha\rangle$.
(2) $\hat{\rho}$ is a number state $|n\rangle\langle n|$.

Exercise 8.5. If we care about the means and the variances only, it is easier to look at the Heisenberg picture:

$$\hat{q}_3 = \tau\hat{q}_1 + r\hat{q}_2 = \frac{1}{\sqrt{2}}(\hat{q}_1 + \hat{q}_2), \qquad \hat{p}_4 = \tau'\hat{p}_1 + r'\hat{p}_2 = \frac{1}{\sqrt{2}}(\hat{p}_1 - \hat{p}_2). \tag{8.40}$$

Use these equations to verify Eqs. (8.38) for an initial coherent state $|\alpha\rangle_1 \otimes |0\rangle_2$ for mode 1 and 2.

8.5. A long pulse is a superposition of short pulses

Dual-homodyne is a complicated setup, requiring two homodyne detectors and one more beam splitter. There is a simpler setup to achieve the same measurement called heterodyne detection, but its principle is a bit more complicated to explain. It involves **one long signal pulse** and **a sequence of quick measurements of the long pulse**, and we'll have to go beyond the simple scenario of only two input pulses and two output pulses.

Forget about any beam splitter for now and just think about pulses in free space. Think of a long pulse, the envelope of which is plotted in the top-left figure of Fig. 8.3. Let $\hat{f}$ be the annihilation operator for this long-pulse mode. So far we've been studying one measurement of one mode, but what if we have a fast detector that can do multiple measurements for the duration of this one long pulse?

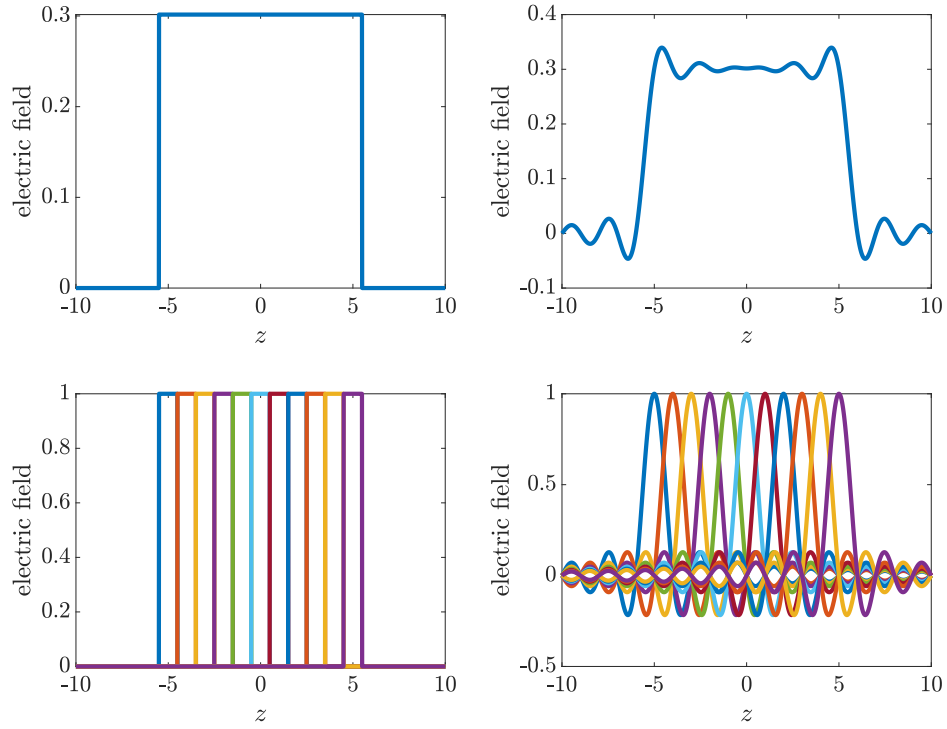

FIGURE 8.3. Top-left: electric-field envelope of a long pulse. Think of the long pulse as a superposition of short pulses at different locations (bottom-left). Right column: variation of the same idea, except that the short pulses are sinc functions. Note that these are **envelopes** of the pulses; the electric fields of optical pulses are obtained by multiplying the envelopes by the rapid oscillations $\exp(ik_0 z)$ (not shown in these plots), or $\exp(-ick_0 t) = \exp(-i\omega_0 t)$ if we adopt the time-domain formalism in Sec. 6.4.

The way forward is to think of **the long pulse as a superposition of M short pulses**, and then we can assume that the fast detector measures the short pulses one-by-one.

First define a set of M short-pulse modes with annihilation operators $\{\hat{b}_l\}$ in the way described in Sec. 3.5.2. We assume the usual commutation relations

$$[\hat{b}_l, \hat{b}_m] = 0, \qquad [\hat{b}_l, \hat{b}_m^\dagger] = \delta_{lm}. \tag{8.41}$$

Each mode is assumed to have a $(\boldsymbol{k}, s)$-space amplitude given by W_{jl}. Suppose that the electric field of each short pulse (recall Eq. (3.91)) looks like

$$\boldsymbol{v}_l(\boldsymbol{r}) \equiv \sum_j \omega_j^{1/2} W_{jl} \boldsymbol{u}_j(\boldsymbol{r}) \propto \text{rect}\left(\frac{z - z_l}{\Delta z}\right) \exp(ik_0 z). \tag{8.42}$$

This rectangle function for various centers z_l is plotted in the bottom-left figure of Fig. 8.3, without the $\exp(ik_0 z)$ factor. (We don't have to use the rect function; it's just clearer to assume something specific here; a variaton of the same idea is shown on the right column.) In classical optics, if we excite these short-pulse modes with **the same amplitude**, say, $\alpha/\sqrt{M}$, then we expect to see a long pulse with electric field

$$\sum_l \frac{\alpha}{\sqrt{M}} \boldsymbol{v}_l(\boldsymbol{r}) \propto \frac{\alpha}{\sqrt{M}} \exp(ik_0 z) \sum_l \text{rect}\left(\frac{z - z_l}{\Delta z}\right). \tag{8.43}$$

The envelope $\frac{1}{\sqrt{M}} \sum_l \text{rect}\left[(z - z_l)/\Delta z\right]$ is plotted in the top-left figure of Fig. 8.3, confirming that it indeed looks like a long pulse. In quantum optics, we can construct a coherent state with these properties by assuming the displacement operator

$$\boxed{\hat{D} = \exp\left(\sum_l \frac{\alpha}{\sqrt{M}} \hat{b}_l^\dagger - \text{H.c.}\right),} \tag{8.44}$$

which excites each short-pulse mode by the same amplitude $\alpha/\sqrt{M}$. We expect $\hat{D}\,|\text{vac}\rangle$ to be the coherent state with a long-pulse mode as its excited mode. To confirm this intuition, we stare at Eq. (8.44) and ask what the excited-mode annihilation operator is. After staring for a while, you should see that it can be rewritten as

$$\boxed{\hat{D} = \exp\Big(\alpha \hat{f}^\dagger - \text{H.c.}\Big),} \qquad \boxed{\hat{f} \equiv \frac{1}{\sqrt{M}} \sum_l \hat{b}_l.} \tag{8.45}$$

We can check that $\hat{f}$ obeys the standard commutation relation $[\hat{f}, \hat{f}^\dagger] = 1$, so it is a bona-fide annihilation operator for the excited mode of the coherent state $\hat{D}\,|\text{vac}\rangle$. Eq. (8.45) also shows that the amplitude of the excited mode is α.

We now work backwards to double-check the electric field of the mode defined by $\hat{f}$. Write $\hat{f}$ in terms of the original $\{\hat{a}_j\}$ for the sinusoidal modes as

$$\hat{f} = \frac{1}{\sqrt{M}} \sum_l \hat{b}_l = \frac{1}{\sqrt{M}} \sum_l \sum_j W_{jl}^* \hat{a}_j = \sum_j \underbrace{\left(\frac{1}{\sqrt{M}} \sum_l W_{jl}^*\right)}_{\equiv \tilde{W}_j^*} \hat{a}_j. \tag{8.46}$$

This expression shows that the $(\boldsymbol{k}, s)$-space amplitude of the excited mode is

$$\tilde{W}_j \equiv \frac{1}{\sqrt{M}} \sum_l W_{jl}. \tag{8.47}$$

Recall from Eq. (3.91) that the electric field given a $(\boldsymbol{k}, s)$-space amplitude $\tilde{W}_j$ for a mode is proportional to $\sum_j \omega_j^{1/2} \tilde{W}_j \boldsymbol{u}_j(\boldsymbol{r})$. For our $\tilde{W}_j$, the electric field becomes

$$\sum_j \omega_j^{1/2} \tilde{W}_j \boldsymbol{u}_j(\boldsymbol{r}) \propto \sum_j \omega_j^{1/2} \left(\frac{1}{\sqrt{M}} \sum_l W_{jl}\right) \boldsymbol{u}_j(\boldsymbol{r}) = \frac{1}{\sqrt{M}} \sum_l \sum_j \omega_j^{1/2} W_{jl} \boldsymbol{u}_j(\boldsymbol{r}) = \frac{1}{\sqrt{M}} \sum_l \boldsymbol{v}_l(\boldsymbol{r}). \tag{8.48}$$

This is a sum of the electric fields $\boldsymbol{v}_l(\boldsymbol{r})$ of the short-pulse modes given by Eq. (8.42). It is given by

$$\frac{1}{\sqrt{M}} \sum_l \boldsymbol{v}_l(\boldsymbol{r}) \propto \exp(ik_0 z) \sum_l \text{rect}\left(\frac{z - z_l}{\Delta z}\right), \tag{8.49}$$

which is indeed the long pulse we want.

To summarize, a coherent state with a long-pulse mode as its excited mode and α as its amplitude can be rewritten as

$$\boxed{\hat{D}\,|\text{vac}\rangle = \exp\Big(\alpha\hat{f}^\dagger - \text{H.c.}\Big)\,|\text{vac}\rangle = \exp\left(\sum_l \frac{\alpha}{\sqrt{M}}\hat{b}_l^\dagger - \text{H.c.}\right)|\text{vac}\rangle\,,} \tag{8.50}$$

where

(1) $\hat{f}$ is the annihilation operator of the long-pulse mode.
(2) α is the amplitude of the long-pulse mode.
(3) $\{\hat{b}_l\}$ are the annihilation operators of the short-pulse modes.
(4) The amplitudes of the short-pulse modes are given by

$$\begin{pmatrix} \alpha/\sqrt{M} \\ \vdots \\ \alpha/\sqrt{M} \end{pmatrix}. \tag{8.51}$$

The derivation is a bit long-winded but hopefully this end result makes sense to you. In classical optics, it is obvious that a long pulse is a superposition of short pulses. In quantum optics, we need to be a bit more specific about the mode operators and the state. It's easier if we can assume a coherent state and work with the displacement operator.

Exercise 8.6. Suppose that we transform the M short-pulse modes to M new modes, and the long-pulse mode is one of the latter, i.e., let

$$\hat{f}_m = \sum_l C_{ml}\hat{b}_l, \qquad C_{11} = C_{12} = \cdots = C_{1M} = \frac{1}{\sqrt{M}}, \tag{8.52}$$

where $\hat{f}_1$ is the $\hat{f}$ defined earlier and C is a unitary matrix. Use the formalism in Sec. 5.1.2 to rederive Eq. (8.50).

8.6. Heterodyne detection

Now that we know how to rewrite a long-pulse coherent state as a coherent state with M short pulses, it becomes clear how we can measure both quadratures of α: perform a sequence of homodyne measurements of the short-pulse modes, with **varying local-oscillator phases** to measure different quadratures of the different short pulses in the signal. This is precisely what heterodyne detection does; see Fig. 8.4 for the experimental setup.

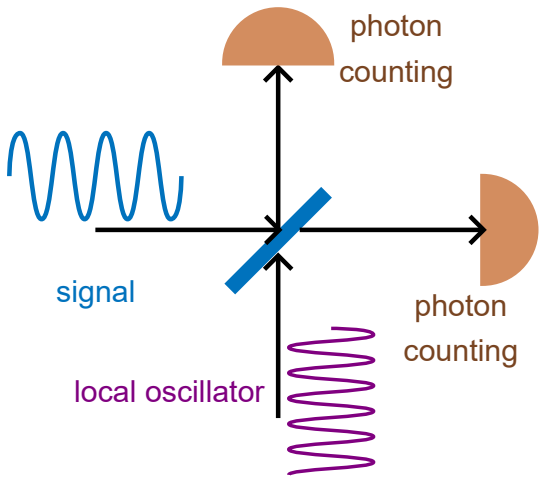

FIGURE 8.4. Setup of heterodyne detection. It's the same as homodyne, except that the local oscillator has a slightly different center frequency $\omega_0 + \Omega$. (The difference in the frequencies is greatly exaggerated in the figure.)

We will adopt the time-domain convention for pulses in Sec. 6.4 from now on. In heterodyne detection, the local oscillator is also a long optical pulse, but now its phase varies across the multiple short-pulse modes. Let

$$t_m = m\Delta t, \quad m = 0, \dots, M-1, \tag{8.53}$$

be the center positions of the M short pulses in the local oscillator. Suppose that the electric field of the local oscillator looks like

$$\alpha_0 e^{-i\omega_0 t} \sum_m e^{-i\Omega t_m} \operatorname{rect}\left(\frac{t-t_m}{\Delta t}\right), \tag{8.54}$$

where α_0 is a complex constant, so that the phases of the short-pulse modes vary as $\angle\alpha_0 - \Omega t_m$. The amplitudes of the short pulse modes for the local oscillator are then given by

$$\alpha_2(t_m) \propto \alpha_0 \exp(-i\Omega t_m). \tag{8.55}$$

This time-varying phase is typically imposed by shifting the center frequency of the local oscillator slightly from ω_0 to $\omega_0 + \Omega$, so that the electric field would look like

$$e^{-i\omega_0 t - i\Omega t} \sum_m \operatorname{rect}\left(\frac{t-t_m}{\Delta t}\right) \approx e^{-i\omega_0 t} \sum_m e^{-i\Omega t_m} \operatorname{rect}\left(\frac{t-t_m}{\Delta t}\right). \tag{8.56}$$

Ω is usually a radio frequency (MHz to GHz) in practice.

Side note. *"Hetero" in the word heterodyne means "different" and refers to the center frequency $\omega_0 + \Omega$ of the local oscillator being different from ω_0 of the signal.*

The short-pulse modes of the local oscillator interfere with the short-pulse modes of the signal one by one at the beam splitter. The input-output relation should now be expressed as

$$\begin{pmatrix} \hat{a}_3(T+t_m) \\ \hat{a}_4(T+t_m) \end{pmatrix} = \begin{pmatrix} \hat{U}^\dagger(t_m)\hat{a}_3(T)\hat{U}(t_m) \\ \hat{U}^\dagger(t_m)\hat{a}_4(T)\hat{U}(t_m) \end{pmatrix} = S \begin{pmatrix} \hat{U}^\dagger(t_m)\hat{a}_1(0)\hat{U}(t_m) \\ \hat{U}^\dagger(t_m)\hat{a}_2(0)\hat{U}(t_m) \end{pmatrix} = S \begin{pmatrix} \hat{a}_1(t_m) \\ \hat{a}_2(t_m) \end{pmatrix}, \quad m = 0, 1, 2, \dots \tag{8.57}$$

The meaning of this equation is that the input-output relation remains the same for sequences of pulses; $\hat{a}_1(t_m)$ and $\hat{a}_2(t_m)$ should now be regarded as the annihilation operators for short-pulse modes in the input arms in the sense of Sec. 6.4. We measure the photon numbers $\hat{a}_3^\dagger(T+t_m)\hat{a}_3(T+t_m)$ and $\hat{a}_4^\dagger(T+t_m)\hat{a}_4(T+t_m)$ at each t_m and subtract one from the other to obtain a quadrature operator in terms of $\hat{a}_1(t_m)$. For a signal in the coherent state, we know the probability density of each outcome x_m from Sec. 8.3. With the outcome suitably scaled, the probability density is the same as that for a quadrature measurement given by Eq. (4.7). Let the observable being measured be Eq. (8.14) divided by some constant C, so that it can be expressed as

$$\hat{O}(t_m) \equiv \frac{1}{C}\left[\hat{a}_3^\dagger(T+t_m)\hat{a}_3(T+t_m) - \hat{a}_4^\dagger(T+t_m)\hat{a}_4(T+t_m)\right] \tag{8.58}$$

$$= \frac{1}{\sqrt{2}}\left[e^{-i\phi_m}\hat{a}_1(t_m) + \text{H.c.}\right], \qquad \boxed{\phi_m \equiv \theta + \angle\alpha_0 - \Omega t_m,} \tag{8.59}$$

coinciding with the usual definition of a quadrature operator in this book. The phase ϕ_m depends on the local-oscillator phase $\angle\alpha_0 - \Omega t_m$ and also the θ defined by Eq. (8.11), which comes from the optics. Since each short-pulse mode of the signal has amplitude $\alpha/\sqrt{M}$, as we derived in Sec. 8.5, the mean of $\hat{O}(t_m)$ is given by

$$\langle O(t_m)\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\phi_m}\frac{\alpha}{\sqrt{M}} + \text{c.c.}\right) = \sqrt{\frac{2}{M}}\operatorname{Re}\left(\alpha e^{-i\phi_m}\right). \tag{8.60}$$

The M outcomes are independent random variables, since the coherent state is a tensor product of coherent states in terms of the short-pulse modes and we are measuring those modes independently one by one. The probability

density for all the outcomes is hence

$$\boxed{f(x_1,\ldots,x_M|\alpha) = \frac{1}{\pi^{M/2}} \exp\left\{-\sum_m \left[x_m - \sqrt{\frac{2}{M}}\,\mathrm{Re}\left(\alpha e^{-i\phi_m}\right)\right]^2\right\}.} \tag{8.61}$$

The outcomes form a **noisy time series**:

(1) their averages $\propto \mathrm{Re}\left(\alpha e^{-i\phi_m}\right)$ oscillate at the frequency Ω with respect to discrete time t_m because $\phi_m = \phi_0 - \Omega t_m$;
(2) there's also noise because each outcome is an independent Gaussian random variable with variance $1/2$.

Let's come back to the communication scenario discussed in Sec. 8.4. We have M real numbers $(x_1,\ldots,x_M)$ coming out of the measurements, but there are, after all, only two real parameters $\mathrm{Re}\,\alpha$ and $\mathrm{Im}\,\alpha$ that we want to estimate. Is there any way of simplifying the outcomes? A bit of statistics is necessary to derive the best procedure, but I'll skip the derivation and just tell you the end result: Given the measurement outcomes $(x_1,\ldots,x_M)$, we should compute

$$y_1 \equiv \sqrt{\frac{2}{M}} \sum_m x_m \cos\phi_m, \qquad\qquad y_2 \equiv \sqrt{\frac{2}{M}} \sum_m x_m \sin\phi_m. \tag{8.62}$$

This procedure is called **demodulation**. With some benign assumptions (see Exercise 8.7), it can be shown that the probability density of (y_1, y_2) is

$$\boxed{f'(y_1,y_2|\alpha) = \frac{1}{\pi}\exp\left[-(y_1 - \mathrm{Re}\,\alpha)^2 - (y_2 - \mathrm{Im}\,\alpha)^2\right].} \tag{8.63}$$

This is exactly the same as Eq. (8.26) from dual-homodyne! At the end of the day, heterodyne together with demodulation gives exactly the same probability density as that from dual-homodyne for a coherent state, and by the Sudarshan trick, the probability densities from the two methods are also the same and given by Eq. (8.34) for an arbitrary signal state.

The theory of heterodyne detection is complicated, but the experimental setup is significantly simpler than dual-homodyne—it's the same as one homodyne, except that the local oscillator has a slightly different center frequency. Shifting the laser frequency is easy with an optical modulator (acousto-optic or electro-optic). In quantum optics, it's extremely important to minimize loss in your setup (because of quantum dissipation-fluctuation relations), so it's always good to use fewer optical components. Demodulation is trivial with an oscilloscope or a computer.

Another practical advantage of heterodyne is that the outcomes form a time series oscillating at the frequency Ω, typically a radio frequency. The time series is carried as an electric signal in the detector and the electronics before it is recorded permanently in data storage, so additional electronic noise may still be added to it before it's recorded. Electronic noise often falls off like $1/f$ in the frequency domain, so a high-frequency electric signal will suffer less from the $1/f$ noise.

One small shortcoming of heterodyne is that, for a signal pulse mode of the same duration, it requires a faster detector to perform the sequence of quick measurements to capture information about both quadratures. A minimum of $M = 2$ is necessary, so the detector is required to be at least twice as fast as the detectors for dual-homodyne.

Exercise 8.7. An alternative way of writing Eq. (8.61) is to assume that each outcome is a random variable given by

$$X_m = \bar{X}_m + Z_m, \qquad\qquad \bar{X}_m \equiv \sqrt{\frac{2}{M}}\,\mathrm{Re}\left(\alpha e^{-i\phi_m}\right), \tag{8.64}$$

where $\{Z_m\}$ are independent zero-mean Gaussian random variables, each with variance $1/2$.

(1) Show that

$$\bar{X}_m = \sqrt{\frac{2}{M}}[(\mathrm{Re}\,\alpha)\cos\phi_m + (\mathrm{Im}\,\alpha)\sin\phi_m]. \tag{8.65}$$

(2) Assume

$$\Omega = \frac{\pi L}{M\Delta t}, \tag{8.66}$$

where L is a nonzero integer and $|L| < M$. (This assumption simplifies the math a bit. It means that, over the duration $M\Delta t$ of the long pulse, the phase of the local oscillator covers the range from ϕ_0 to $\phi_0 - \Omega t_M = \phi_0 - \pi L$ (Fig. 8.5), while $|L| < M$ ensures that $|\Omega\Delta t| = \pi|L|/M \neq \pi$, so that the local-oscillator phase doesn't vary in increments of π and the measurements don't end up measuring one quadrature only.)

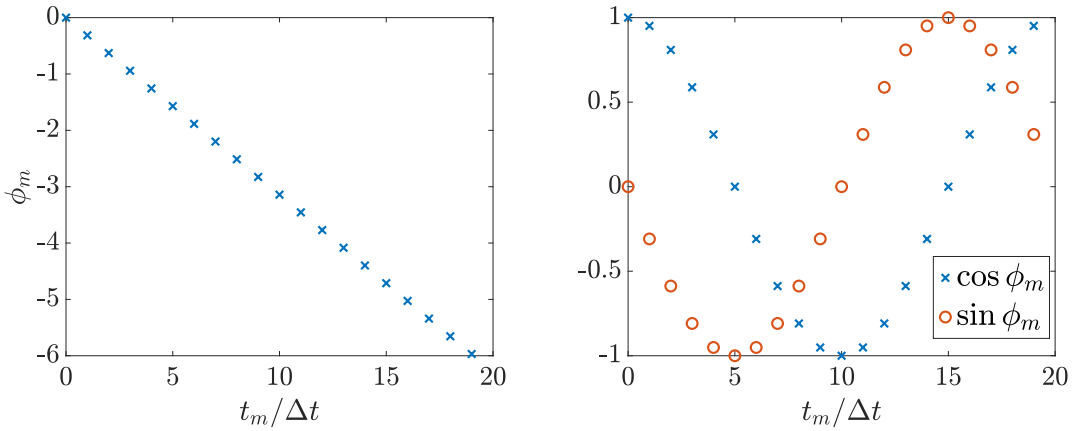

FIGURE 8.5. Left: a plot of the local-oscillator phase ϕ_m versus t_m (normalized by the duration of the short pulse Δt), assuming $\phi_0 = 0$, $L = 2$, $M = 20$. The phase goes from 0 to -2π in this example. Right: a plot of $\cos\phi_m$ and $\sin\phi_m$ versus t_m.

Show that

$$\sum_{m=0}^{M-1} \cos^2\phi_m = \frac{M}{2}, \qquad \sum_{m=0}^{M-1} \sin^2\phi_m = \frac{M}{2}, \qquad \sum_{m=0}^{M-1} (\sin\phi_m)(\cos\phi_m) = 0. \tag{8.67}$$

(3) Show that

$$Y_1 \equiv \sqrt{\frac{2}{M}} \sum_{m=0}^{M-1} X_m \cos\phi_m \qquad Y_2 \equiv \sqrt{\frac{2}{M}} \sum_{m=0}^{M-1} X_m \sin\phi_m \tag{8.68}$$

are Gaussian random variables, with statistics

$$\mathbb{E}(Y_1) = \mathrm{Re}\,\alpha, \qquad \mathbb{E}(Y_2) = \mathrm{Im}\,\alpha, \qquad \mathbb{V}(Y_1) = \mathbb{V}(Y_2) = \frac{1}{2}, \qquad \mathrm{COV}(Y_1, Y_2) = 0, \tag{8.69}$$

so that their probability density is given by Eq. (8.63).

(4) Prove that the outcomes Y_1, Y_2 from the demodulation are **sufficient statistics** about $\mathrm{Re}\,\alpha$ and $\mathrm{Im}\,\alpha$ (https://en.wikipedia.org/wiki/Sufficient_statistic). (This means that we haven't lost any information about α through the demodulation.)

Side note. *A lot of the concepts we use to study heterodyne detection, such as demodulation, noisy time series, and sufficient statistics, come from electrical engineering and statistics. There is a long history of electrical engineers and statisticians studying quantum optics, and they have brought those techniques to the field.*

Exercise 8.8. We mentioned earlier that dual-homodyne is a generalized measurement and an ancilla is involved. What is the ancilla in heterodyne detection?

CHAPTER 9

Michelson and Mach-Zehnder Interferometers

9.1. Introduction

The detection of gravitational waves by optical interferometers at LIGO (Laser Interferometer Gravitational-Wave Observatory, https://www.youtube.com/watch?v=z7pKXVkcDzs, https://www.ligo.caltech.edu/page/ligo-gw-interferometer) is the most useful application of quantum optics, and arguably the only useful application of quantum optics so far. LIGO scientists have been able to remove so many other noise sources, such as seismic noise and thermal vibrations of the mirrors, that the quantum shot noise has emerged as a significant problem. A quantum treatment becomes necessary to study it and deal with it.

The type of interferometer they use is called a **Michelson** interferometer. Here we will study a simple version of it. Its physics turns out to be the same as another type called the **Mach-Zehnder** interferometer so we will study them together.

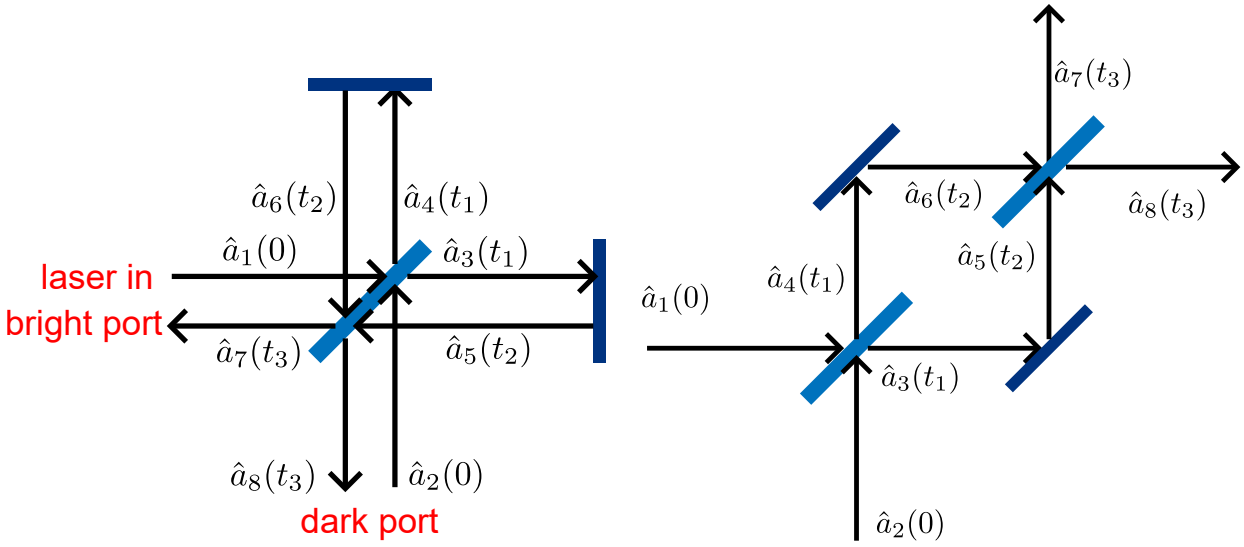

FIGURE 9.1. Left: A Michelson interterometer. Right: A Mach-Zehnder interferometer.

Figure 9.1 shows the two types of interferometers. The input-output relations are the same for both, even though the experimental setups differ. We will study them using the **Heisenberg picture**, since everything consists of passive linear optics and we usually care about the expected values and variances of the outputs only, both of which are pretty easy to compute with the Heisenberg picture.

9.2. Input-output relations

Assume that there are two pulse modes going into the first beam splitter and their annihilation operators are $\hat{a}_1(0)$ and $\hat{a}_2(0)$, respectively. As we learned in Chapter 6, if the beam splitter is lossless, we can write the input-output relation as

$$\boxed{\begin{pmatrix}\hat{a}_3(t_1)\\ \hat{a}_4(t_1)\end{pmatrix} = S\begin{pmatrix}\hat{a}_1(0)\\ \hat{a}_2(0)\end{pmatrix},} \tag{9.1}$$

where S is the scattering matrix.

The two output pulses then go their separate ways in the two **arms** of the interferometer. The important feature of an interferometer is that the two pulses may experience two different **phase shifts** in the two arms. For example, the arm lengths may be different, or there may be phase modulators in the two arms. In a gravitational-wave detector, a gravitational wave acts as a classical force that moves the mirrors in the Michelson interferometer, so that the arm lengths differ slightly, on the order of 10^{-19} m.

First, let us assume that there is no phase shift in either arm, the arm lengths are identical and given by L. Let

$$t_2 - t_1 = L/c \tag{9.2}$$

be the time it takes for the pulses to propagate through the arms. Let $\hat{a}_5(t_2)$ be the annihilation operator for the pulse mode at the end of the first arm, and $\hat{a}_6(t_2)$ be the annihilation operator for the pulse mode at the end of the second arm. From Sec. 6.3, we learned that the input-output relation for pulse propagation looks like

$$\hat{f}(z_l, t_2) = \hat{f}(z_l - c(t_2 - t_1), t_1) = \hat{f}(z_l - L, t_1) \tag{9.3}$$

for a propagation distance of $L = c(t_2 - t_1)$. If we assume that $\hat{f}(z_l - L, t_1)$ is $\hat{a}_3(t_1)$ at the entrance of the first arm and $\hat{f}(z_l, t_2)$ is $\hat{a}_5(t_2)$ at the exit of the first arm, then we'd have

$$\hat{a}_5(t_2) = \hat{a}_3(t_1). \tag{9.4}$$

Similarly, in the second arm, we'd have

$$\hat{a}_6(t_2) = \hat{a}_4(t_1). \tag{9.5}$$

There are mirrors in the arms in practice and the pulses don't travel in only one direction, but it turns out that the relations above still hold as long as we treat L as the total distance each pulse has to propagate from the entrance to the exit.

Suppose now that there is a change ΔL_1 to the length of the first arm. Let's assume that input operator

$$\hat{a}_3(t_1) = \hat{f}(z_l - L, t_1) \tag{9.6}$$

is the same as before, but the output operator, because of the length change, should be set as

$$\hat{a}_5(t_2) = \hat{f}(z_l + \Delta L_1, t_2), \tag{9.7}$$

so that the difference between the two positions is $(z_l + \Delta L_1) - (z_l - L) = L + \Delta L_1$, which is the new length of the arm. When ΔL is much shorter than the length of the pulse, it turns out that the input-output relation can be approximated as

$$\hat{a}_5(t_2) \approx e^{ik_0 \Delta L_1} \hat{f}(z_l, t_2) = e^{ik_0 \Delta L_1} \hat{a}_3(t_1). \tag{9.8}$$

This phase shift due to length change is a well known result in classical optics, but in case you are not familiar with it, Sec. 9.2.1 offers a derivation using our formalism. By the same argument, if there is a change ΔL_2 to the length of the second arm, we have

$$\hat{a}_6(t_2) \approx e^{ik_0 \Delta L_2} \hat{a}_4(t_1). \tag{9.9}$$

In matrix form,

$$\boxed{\begin{pmatrix} \hat{a}_5(t_2) \\ \hat{a}_6(t_2) \end{pmatrix} = \begin{pmatrix} e^{i\phi_1} & 0 \\ 0 & e^{i\phi_2} \end{pmatrix} \begin{pmatrix} \hat{a}_3(t_1) \\ \hat{a}_4(t_1) \end{pmatrix},} \qquad \boxed{\phi_1 \equiv k_0 \Delta L_1,} \qquad \boxed{\phi_2 \equiv k_0 \Delta L_2,} \tag{9.10}$$

where ϕ_1 and ϕ_2 are the phase shifts in the first and second arms, respectively.

Finally, the pulses go through a beam splitter again. Assume that the second beam splitter has a scattering matrix $\tilde{S}$, such that

$$\boxed{\begin{pmatrix} \hat{a}_7(t_3) \\ \hat{a}_8(t_3) \end{pmatrix} = \tilde{S} \begin{pmatrix} \hat{a}_5(t_2) \\ \hat{a}_6(t_2) \end{pmatrix}.} \tag{9.11}$$

Putting Eqs. (9.1), (9.10) and (9.11) together, the final result is

$$\boxed{\begin{pmatrix}\hat{a}_7(t_3)\\ \hat{a}_8(t_3)\end{pmatrix} = \tilde{S}\begin{pmatrix}e^{i\phi_1} & 0\\ 0 & e^{i\phi_2}\end{pmatrix} S\begin{pmatrix}\hat{a}_1(0)\\ \hat{a}_2(0)\end{pmatrix}.} \tag{9.12}$$

9.2.1. Side note: Derivation of Eq. (9.8). Recall from Sec. 6.3 that $\hat{f}(z_l, 0)$ for a pulse mode depends on z_l through the phase $\exp(-ik_z z_l)$ in the $(\boldsymbol{k}, s)$-space amplitude:

$$\hat{f}(z_l, 0) = \sum_j W^*_{jl}\hat{a}_j, \qquad W_{jl} \propto \text{rect}\left(\frac{k_z - k_0}{\kappa}\right)\exp(-ik_z z_l). \tag{9.13}$$

If z_l is displaced to $z_l + \Delta L$, we have a new $(\boldsymbol{k}, s)$-space amplitude given by

$$\hat{f}(z_l + \Delta L, 0) = \sum_j \tilde{W}^*_{jl}\hat{a}_j, \quad \tilde{W}_{jl} \propto \text{rect}\left(\frac{k_z - k_0}{\kappa}\right)\exp[-ik_z(z_l + \Delta L)] = W_{jl}\exp(-ik_z\Delta L). \tag{9.14}$$

Now we make the assumption

$$\boxed{\kappa\Delta L \ll 1.} \tag{9.15}$$

Recall that the pulse width is $\propto 1/\kappa$, so this assumption means that the displacement ΔL is much smaller than the pulse width. The function $\text{rect}[(k_z - k_0)/\kappa]$ implies that we care about $k_z \in [k_0 - \kappa/2, k_0 + \kappa/2]$ only. Write

$$\exp(-ik_z\Delta L) = \exp(-ik_0\Delta L)\exp[-i(k_z - k_0)\Delta L], \tag{9.16}$$

and notice that the phase $(k_z - k_0)\Delta L$ in the second exponential changes from $-\kappa\Delta L/2$ to $\kappa\Delta L/2$. When $\kappa\Delta L \ll 1$, $|(k_z - k_0)\Delta L| \le \kappa\Delta L/2$ is close to zero for the whole range of k_z, so $\exp[-i(k_z - k_0)\Delta L] \approx 1$, and we can assume

$$\boxed{\text{rect}\left(\frac{k_z - k_0}{\kappa}\right)\exp(-ik_z\Delta L) \approx \text{rect}\left(\frac{k_z - k_0}{\kappa}\right)\exp(-ik_0\Delta L).} \tag{9.17}$$

In other words, the rectangle function $\text{rect}[(k_z - k_0)/\kappa]$ is so sharp around $k_z = k_0$ and $\exp(-ik_z\Delta L)$ varies so slowly that the rectangle behaves like a Dirac delta function and we can assume $k_z \approx k_0$ in the exponential; see Fig. 9.2 for an illustration. For example, if a pulse is around 1 μs long in time, then it'd be around $2\pi/\kappa = 300$ m long in space. The displacement ΔL, on the other hand, is typically much shorter than the wavelength, which is around 1 μm usually, so our approximation is excellent.

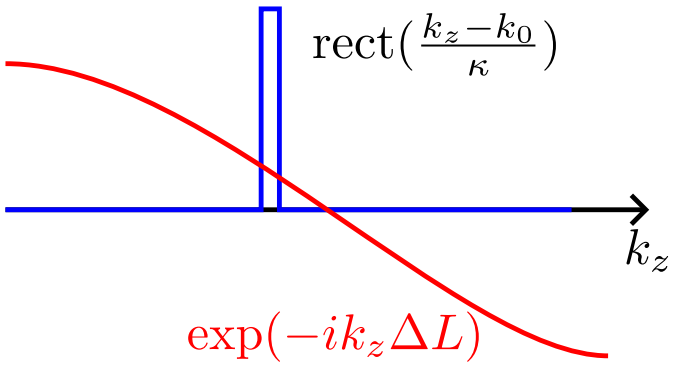

FIGURE 9.2. If $\kappa\Delta L \ll 1$, then the rectangle function is so sharp relative to $\exp(-ik_z\Delta L)$ that the latter can be approximated as $\exp(-ik_0\Delta L)$.

Putting this approximation in Eq. (9.14), we obtain

$$\tilde{W}_{jl} \approx W_{jl} \exp(-ik_0 \Delta L), \tag{9.18}$$

$$\hat{f}(z_l + \Delta L, 0) \approx \sum_j W^*_{jl} e^{ik_0 \Delta L} \hat{a}_j = e^{ik_0 \Delta L} \hat{f}(z_l, 0). \tag{9.19}$$

Now we apply this approximation on Eqs. (9.6) and (9.7) to obtain

$$\hat{a}_5(t_2) \equiv \hat{f}(z_l + \Delta L_1, t_2) \approx e^{ik_0 \Delta L_1} \hat{f}(z_l, t_2) = e^{ik_0 \Delta L_1} \hat{f}(z_l - L, t_1) = e^{ik_0 \Delta L_1} \hat{a}_3(t_1). \tag{9.20}$$

As before, we don't have to use the rectangle function; any function that has a center at k_0 and a width of κ can work.

9.3. Output dependence on phase shift

To be concrete, let's assume

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \qquad \tilde{S} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{9.21}$$

The input-output relation becomes

$$\begin{pmatrix} \hat{a}_7(t_3) \\ \hat{a}_8(t_3) \end{pmatrix} = e^{i\bar{\phi}} \begin{pmatrix} \cos\left(\frac{\phi_1 - \phi_2}{2}\right) & i \sin\left(\frac{\phi_1 - \phi_2}{2}\right) \\ i \sin\left(\frac{\phi_1 - \phi_2}{2}\right) & \cos\left(\frac{\phi_1 - \phi_2}{2}\right) \end{pmatrix} \begin{pmatrix} \hat{a}_1(0) \\ \hat{a}_2(0) \end{pmatrix}, \qquad \bar{\phi} \equiv \frac{1}{2}(\phi_1 + \phi_2). \tag{9.22}$$

If $\phi_1 = \phi_2$,

$$\hat{a}_7(t_3) = e^{i\bar{\phi}} \hat{a}_1(0), \qquad \hat{a}_8(t_3) = e^{i\bar{\phi}} \hat{a}_2(0), \tag{9.23}$$

meaning that the first input goes to the first output, and the second input goes to the second output.

Now assume that a laser beam in a coherent state $|\alpha\rangle$ goes into the first input and nothing (i.e., vacuum state $|0\rangle$) goes into the second input. If $\phi_1 = \phi_2$, the laser beam will come out of the first output, and nothing (vacuum) comes out of the second output. This is why the first input and output (with operators $\hat{a}_1(0)$ and $\hat{a}_7(t_3)$) are called the **bright ports**, while the second input and output (with operators $\hat{a}_2(0)$ and $\hat{a}_8(t_3)$) are called the **dark ports**. To put it another way, the laser beam is split evenly into the two arms, and when the two beams come back to a beam splitter, they constructively interfere at the bright output port, and destructively interfere at the dark output port.

$\phi_1 \neq \phi_2$ is, of course, the interesting case. We have

$$\hat{a}_7(t_3) = e^{i\bar{\phi}} \left[\hat{a}_1(0) \cos\left(\frac{\phi_1 - \phi_2}{2}\right) + i\hat{a}_2(0) \sin\left(\frac{\phi_1 - \phi_2}{2}\right) \right], \tag{9.24}$$

$$\hat{a}_8(t_3) = e^{i\bar{\phi}} \left[i\hat{a}_1(0) \sin\left(\frac{\phi_1 - \phi_2}{2}\right) + \hat{a}_2(0) \cos\left(\frac{\phi_1 - \phi_2}{2}\right) \right]. \tag{9.25}$$

Notice that the dark port now has a nonzero mean field given by

$$\langle \hat{a}_8(t_3) \rangle = e^{i\bar{\phi}} i\alpha \sin\left(\frac{\phi_1 - \phi_2}{2}\right). \tag{9.26}$$

Because of the relative phase shift in the two arms, there is **incomplete destructive interference** at the dark port, and some light leaks out. By measuring the dark port, one can **estimate** the relative phase shift $\phi_1 - \phi_2$. This is the basic principle of optical interferometry for phase estimation.

The relative phase shift is typically miniscule, so we can assume

$$|\phi_1 - \phi_2| \ll 1, \tag{9.27}$$

which allows us to make the first-order Taylor approximation

$$\cos\left(\frac{\phi_1 - \phi_2}{2}\right) \approx 1, \qquad \sin\left(\frac{\phi_1 - \phi_2}{2}\right) \approx \frac{\phi_1 - \phi_2}{2}. \tag{9.28}$$

If we also make the classical approximation $\hat{a}_1(0) \approx \alpha$ for the first input, we obtain

$$\hat{a}_7(t_3) \approx e^{i\bar{\phi}}\left[\alpha + i\hat{a}_2(0)\frac{\phi_1-\phi_2}{2}\right], \tag{9.29}$$

$$\boxed{\hat{a}_8(t_3) \approx e^{i\bar{\phi}}\left[i\alpha\frac{\phi_1-\phi_2}{2} + \hat{a}_2(0)\right].} \tag{9.30}$$

Notice that the mean outputs are given by

$$\langle \hat{a}_7(t_3)\rangle \approx e^{i\bar{\phi}}\alpha, \qquad \langle \hat{a}_8(t_3)\rangle \approx e^{i\bar{\phi}} i\alpha\frac{\phi_1-\phi_2}{2}, \tag{9.31}$$

so the bright port isn't sensitive to the relative phase shift in the first order and it doesn't hurt if we don't measure it. Eq. (9.30) for the dark-port output, on the other hand, is the key result of this chapter. We should interpret it as a **quantum dissipation-fluctuation relation** and $\hat{a}_2(0)$ as a quantum noise term. This dependence on $\hat{a}_2(0)$ shows that **the noise ultimately comes from the dark input port**, as first discovered by Caves [12].

Beware that we've ignored any loss in the input-output relation. A more careful analysis including loss can be performed using the model in Chapter 7. There will be an attenuation of the signal as well as additional noise terms.

Exercise 9.1. Verify Eq. (9.22).

Exercise 9.2.

(1) Show that Eq. (9.30) obeys $[\hat{a}_8(t_3), \hat{a}_8^\dagger(t_3)] = 1$. (Despite all the approximations, Eq. (9.30) remains a legal Heisenberg equation of motion.)

(2) Without the approximations, we should write

$$\hat{a}_8(t_3) = e^{i\bar{\phi}}\left[i\sin\left(\frac{\phi_1-\phi_2}{2}\right)\hat{a}_1(0) + \cos\left(\frac{\phi_1-\phi_2}{2}\right)\hat{a}_2(0)\right]. \tag{9.32}$$

   (a) Show that $\left[\hat{a}_8(t_3), \hat{a}_8^\dagger(t_3)\right] = 1$.

   (b) Given the $\hat{O}$ in Eq. (9.33), find its variance if the first input is a coherent state and the second input is a vacuum state.

   (c) If $|\phi_1 - \phi_2| \ll 1$, show that the variance of $\hat{O}$ is determined mostly by the second input.

Exercise 9.3. Another use of a Mach-Zehnder interferometer is as an optical switch. Suppose that ϕ_1 and ϕ_2 can be controlled by optical phase modulators in the two arms. Find the minimum $|\phi_1 - \phi_2|$ such that the laser beam comes out completely in the second output, rather than the first output.

9.4. Homodyne detection

Suppose that we measure the dark port by homodyne detection, which measures the observable

$$\hat{O} \equiv \frac{1}{\sqrt{2}}\left[e^{-i\theta}\hat{a}_8(t_3) + \text{H.c.}\right], \tag{9.33}$$

where θ is the local-oscillator phase. Given Eq. (9.30), the mean of the output becomes

$$\langle O\rangle = \frac{1}{\sqrt{2}}\left[e^{-i\theta}e^{i\bar{\phi}}i\alpha\frac{\phi_1-\phi_2}{2} + \text{c.c.}\right] = \frac{1}{\sqrt{2}}(\phi_1-\phi_2)\,\text{Re}(e^{-i\theta}e^{i\bar{\phi}}i\alpha). \tag{9.34}$$

To maximize the sensitivity of the mean to $\phi_1 - \phi_2$, we should set the local-oscillator phase θ such that $|\,\text{Re}(e^{-i\theta}e^{i\bar{\phi}}i\alpha)|$ is maximized. This can be accomplished if

$$\theta = \bar{\phi} + \frac{\pi}{2} + \angle\alpha + 2\pi m, \quad m \text{ is any integer.} \tag{9.35}$$

Then

$$\mathrm{Re}(e^{-i\theta}e^{i\bar{\phi}}i\alpha) = |\alpha|, \qquad \langle O\rangle = \frac{|\alpha|}{\sqrt{2}}(\phi_1 - \phi_2). \tag{9.36}$$

On the other hand, Eq. (9.30) shows that the variance of $\hat{O}$ is equal to the variance of a quadrature of $\hat{a}_2(0)$. Use Eq. (9.30) to write

$$\hat{O} = \frac{|\alpha|}{\sqrt{2}}(\phi_1 - \phi_2) + \hat{O}_2, \qquad \hat{O}_2 \equiv \frac{1}{\sqrt{2}}\Big[e^{-i\theta}e^{i\bar{\phi}}\hat{a}_2(0) + \text{H.c.}\Big]. \tag{9.37}$$

Then

$$\boxed{\langle \Delta O^2\rangle = \langle \Delta O_2^2\rangle = \frac{1}{2},} \tag{9.38}$$

because the dark-port input is in a vacuum state, which has a variance equal to $1/2$ for a quadrature operator $\hat{O}_2$ for any θ (see Exercise 4.26). This variance is called the **shot-noise limit** in interferometry. The SNR becomes

$$\boxed{\text{SNR} = \frac{\langle O\rangle^2}{\langle \Delta O^2\rangle} = |\alpha|^2(\phi_1 - \phi_2)^2.} \tag{9.39}$$

We can increase the SNR if we increase the average photon number $|\alpha|^2$ of the laser in each pulse mode, but there would be other issues when the laser power is too high. For example, the mirrors are not perfect in practice and may absorb a tiny fraction of the light. When the laser power is too high, the absorbed energy can turn into random mechanical fluctuations on the mirror surface.

LIGO has the problem that they cannot increase the laser power any higher without running into those issues. The solution, first conceived by Caves in 1981 [12] and eventually implemented in LIGO in the 2010s, is to inject into the dark port a different quantum state called a **squeezed state**, which we will study in Chapter 10.

Side note. *In practice, the relative phase shift $\phi_1 - \phi_2$ varies in time, so one should perform a sequence of measurements to measure the phase shift as a function of time. The properties of the detectors determine the pulse modes being measured, and the rate R of the measurements is related to the duration Δt between two pulse modes via $R = 1/\Delta t$, which is in the range of MHz–GHz in practice. The average photon number $|\alpha|^2$ of the laser is related to the average power $\mathcal{P}$ through the relation*

$$|\alpha|^2 = \frac{1}{\hbar\omega_0}\mathcal{P}\Delta t, \tag{9.40}$$

where $\mathcal{P}\Delta t$ is the average energy in each pulse mode and the $1/\hbar\omega_0$ factor converts the energy to the average photon number. The input-output relation can now be expressed in terms of the discrete time $t_m \equiv m\Delta t$ as

$$\hat{O}(t_m) = \frac{|\alpha|}{\sqrt{2}}[\phi_1(t_m) - \phi_2(t_m)] + \hat{O}_2(t_m), \tag{9.41}$$

*where $\hat{O}_2(t_m)$ is the quadrature operator of an input pulse mode at t_m in the sense of Sec. 6.4. The outputs $(x_0, x_1, \ldots, x_M)$ hence form a **noisy time series**. A standard approach to noise analysis is to perform a Fourier transform of the time series and look at the spectrum in the **frequency domain**. I won't go into details as it'd require too much background knowledge for an undergraduate course; this is simply a disclaimer that the analysis in this book is elementary, and one must be proficient with more advanced time-series and frequency-domain analysis to study statistics seriously for real interferometers.*

Exercise 9.4. Prove that Eq. (9.35) maximizes $\mathrm{Re}(e^{-i\theta}e^{i\bar{\phi}}i\alpha)$.

Exercise 9.5. Assume Eq. (9.30) and the vacuum state for the dark-port input. Find the probability distribution of $\hat{a}_8^\dagger(t_3)\hat{a}_8(t_3)$.

Exercise 9.6. Let O be the outcome from a von Neumann measurement of $\hat{O}$ given by Eqs. (9.37). Assume that the dark-port input is a vacuum state.

(1) Show that O is a Gaussian random variable. Find its mean and its variance.
(2) Let

$$Y = mO + b \tag{9.42}$$

be an unbiased estimator of $\phi_1 - \phi_2$, meaning that its expected value $\mathbb{E}(Y)$ is

$$\mathbb{E}(Y) = \phi_1 - \phi_2. \tag{9.43}$$

Find the real constants m and b.
(3) The SNR is more properly defined in terms of an unbiased estimator as

$$\text{SNR} \equiv \frac{[\mathbb{E}(Y)]^2}{\mathbb{V}(Y)}, \tag{9.44}$$

where $\mathbb{V}(Y)$ is the variance of Y. Show that it agrees with Eq. (9.39).
(4) Repeat the above exercises if the dark-port input is a coherent state with amplitude β. Does the SNR improve?

Exercise 9.7. Suppose that the relative arm-length change $|\Delta L_1 - \Delta L_2|$ is 10^{-19} m. Assume a wavelength of 1 μm for the input laser beam and $\Delta t = 1$ ms (millisecond). Find the average optical power needed to achieve an SNR of 1.

Exercise 9.8. Assume a classical single-mode state

$$\hat{\rho} = \int \Phi(\alpha) \, |\alpha\rangle \langle\alpha| \, d^2\alpha, \tag{9.45}$$

where the Sudarshan representation Φ is a nonnegative probability density. Prove that the variance $\langle \Delta O^2 \rangle$ of a quadrature operator

$$\hat{O} \equiv \frac{1}{\sqrt{2}} \left(e^{-i\theta} \hat{a} + \text{H.c.} \right) \tag{9.46}$$

cannot go below $1/2$.

(This exercise shows that all classical states must obey the shot-noise limit for the variance of a quadrature.)

CHAPTER 10

Squeezing

We learned in Chapter 9 that, to overcome the shot-noise limit in interferometry, we need to lower the variance of a quadrature below $1/2$. Exercise 9.8 shows that such a sub-shot-noise variance is impossible for classical states (those with a nonnegative Sudarshan representation). This chapter shows how a nonclassical state called a squeezed state can achieve this goal. For simplicity, we focus on one mode, and we study the Heisenberg picture first.

10.1. Heisenberg picture

Assume the Hamiltonian

$$\boxed{\hat{H} = \frac{\hbar}{2}\Big(i\xi\hat{a}^{\dagger 2} - i\xi^*\hat{a}^2\Big) = \frac{i\hbar}{2}\Big(\xi\hat{a}^{\dagger 2} - \text{H.c.}\Big),} \tag{10.1}$$

where ξ is a complex number. Notice that it contains $\hat{a}^{\dagger 2}$ and $\hat{a}^2$ terms, so it is no longer the passive linear optics we studied in Chapter 6. Physically, this Hamiltonian can occur in some nonlinear optical material, but we will defer a study of its physical origin until Sec. 10.2. Let's look at the Heisenberg equation of motion for $\hat{a}$:

$$\frac{d\hat{a}(t)}{dt} = -\frac{i}{\hbar}\Big[\hat{a}(t), \hat{H}\Big] = -\frac{i}{\hbar}\hat{U}^\dagger(t)\Big[\hat{a}, \hat{H}\Big]\hat{U}(t) = \xi\hat{a}^\dagger(t). \tag{10.2}$$

We can solve it if we also consider the adjoint

$$\frac{d\hat{a}^\dagger(t)}{dt} = \xi^*\hat{a}(t), \tag{10.3}$$

so that

$$\frac{d^2\hat{a}(t)}{dt^2} = \xi\frac{d\hat{a}^\dagger(t)}{dt} = |\xi|^2\hat{a}(t). \tag{10.4}$$

We know the solution to this differential equation is

$$\hat{a}(t) = \hat{C}\exp(|\xi|t) + \hat{D}\exp(-|\xi|t). \tag{10.5}$$

Matching the initial conditions

$$\hat{a}(0) = \hat{C} + \hat{D} \qquad \frac{d\hat{a}(t)}{dt}\bigg|_{t=0} = \xi\hat{a}^\dagger(0) = |\xi|(\hat{C} - \hat{D}), \tag{10.6}$$

we find

$$\hat{C} = \frac{1}{2}\left[\hat{a}(0) + \frac{\xi}{|\xi|}\hat{a}^\dagger(0)\right], \qquad \hat{D} = \frac{1}{2}\left[\hat{a}(0) - \frac{\xi}{|\xi|}\hat{a}^\dagger(0)\right], \tag{10.7}$$

so

$$\boxed{\hat{a}(t) = \hat{a}(0)\cosh(|\xi|t) + \frac{\xi}{|\xi|}\hat{a}^\dagger(0)\sinh(|\xi|t),} \tag{10.8}$$

$$\cosh X \equiv \frac{1}{2}[\exp(X) + \exp(-X)], \quad \sinh X \equiv \frac{1}{2}[\exp(X) - \exp(-X)]. \tag{10.9}$$

Since $\cosh$ and $\sinh$ grow rapidly for increasing t (and exponentially for $|\xi|t \gg 1$; see Fig. 10.1 for plots), the average amplitude $\langle\hat{a}(t)\rangle$ (under the right initial conditions) can grow as the pulse propagates inside the material.

This suggests that the process can amplify the light, and indeed it turns out to happen in a device called an **optical parametric amplifier (OPA)**.

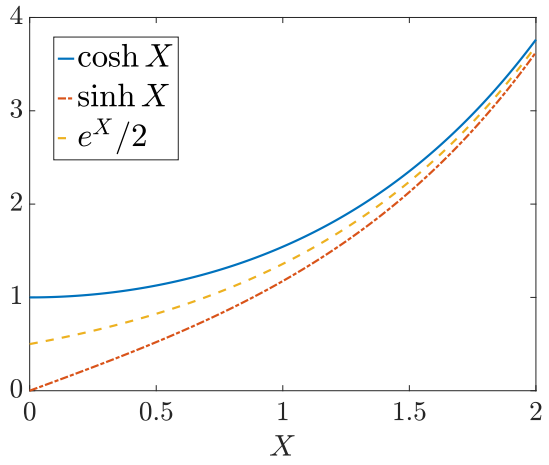

FIGURE 10.1. Plots of hyperbolic functions. $e^X/2$ in-between the two graphs is for comparison.

For our purpose of reducing the shot noise, a more illuminating way of writing the solution is to define two quadrature operators as

$$\boxed{\hat{Q}(t) \equiv \frac{1}{\sqrt{2}}\left[e^{-i\phi}\hat{a}(t) + e^{i\phi}\hat{a}^\dagger(t)\right],} \tag{10.10}$$

$$\boxed{\phi \equiv \frac{1}{2}\angle\xi,} \tag{10.11}$$

$$\boxed{\hat{P}(t) \equiv \frac{1}{\sqrt{2}i}\left[e^{-i\phi}\hat{a}(t) - e^{i\phi}\hat{a}^\dagger(t)\right],} \tag{10.12}$$

so that

$$\boxed{\hat{Q}(t) = \hat{Q}(0)e^{|\xi|t},} \tag{10.13}$$

$$\boxed{\hat{P}(t) = \hat{P}(0)e^{-|\xi|t}.} \tag{10.14}$$

One quadrature grows exponentially, and the other quadrature decays exponentially. The variances become

$$\boxed{\langle\Delta Q^2(t)\rangle = \langle\Delta Q^2(0)\rangle\, e^{2|\xi|t},} \tag{10.15}$$

$$\boxed{\langle\Delta P^2(t)\rangle = \langle\Delta P^2(0)\rangle\, e^{-2|\xi|t}.} \tag{10.16}$$

Equation (10.16), in particular, is precisely what we want for interferometry. If a pulse in a vacuum state goes into a nonlinear material with the Hamiltonian given by Eq. (10.1), then the variance of $\hat{P}$ when the pulse comes out would be reduced below the shot-noise limit $\langle\Delta P^2(0)\rangle = 1/2$. This procedure is called **optical squeezing**. On the other hand, $\langle\Delta Q^2(t)\rangle$ for the other quadrature would grow, and this variance growth is called anti-squeezing. The quadrature to be squeezed can be chosen by picking the right phase for the ξ parameter in the Hamiltonian through Eq. (10.11).

Side note. *For a historical account of the application of optical squeezing to gravitational-wave detectors, see Ref. [9].*

Exercise 10.1. Verify Eqs. (10.2), (10.13), and (10.14).

Exercise 10.2. Check that Eq. (10.8) obeys the commutation relation $[\hat{a}(t), \hat{a}^\dagger(t)] = 1$.

Exercise 10.3. Find $[\hat{Q}(t), \hat{P}(t)]$ from Eqs. (10.13) and (10.14). Show that Eqs. (10.15) and (10.16) still obey the Heisenberg uncertainty relation as long as $\langle \Delta Q^2(0) \rangle$ and $\langle \Delta P^2(0) \rangle$ obey the relation initially.

Exercise 10.4. Compute the average output photon number $\langle \hat{a}^\dagger(t)\hat{a}(t) \rangle$ if the initial state is vacuum.

(Because of this nonzero photon number, the output light is sometimes called spontaneous parametric down conversion (SPDC) or parametric fluorescence. People used to think of it as just amplified spontaneous emission from an amplifier, before realizing in the 1970s that it also leads to squeezing of a quadrature [13, 14].)

Exercise 10.5. If the initial state is vacuum, show that the output state in the Schrödinger picture $|\psi(t)\rangle = \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|0\rangle = \sum_{n=0}^{\infty} \psi_n(t)\,|n\rangle$ contains only number states with even n, i.e., $\psi_n(t) = 0$ if n is odd.

Exercise 10.6. Let $\langle \Delta P^2(0) \rangle = 1/2$. Suppose that, after squeezing, the optical mode experiences loss according to Chapter 7, so that the annihilation operator of the optical mode to be measured is given by

$$\hat{a}_3(T) = \tau \hat{a}(t) + r\hat{a}_2, \tag{10.17}$$

where $\hat{a}(t)$ is given by Eq. (10.8) and $|\tau|^2 + |r|^2 = 1$. Assume that τ is real and the bath (the inaccessible mode 2 in Chapter 7) is in the vacuum state.

(1) Find the variance $\langle \Delta P_3^2 \rangle$ if one measures the squeezed quadrature

$$\hat{P}_3 \equiv \frac{1}{\sqrt{2}i}\left[e^{-i\phi}\hat{a}_3(T) - \text{H.c.}\right] \tag{10.18}$$

after the loss.

(2) The squeezing level in decibel (dB) is defined as

$$R \equiv -10\log_{10}\frac{\langle \Delta P_3^2 \rangle}{\langle \Delta P^2 \rangle_{\text{shot noise}}} = -10\log_{10}\left(2\langle \Delta P_3^2 \rangle\right). \tag{10.19}$$

If $|\tau|^2 = 1$, find R as a function of $|\xi|t$. If $|\tau|^2 < 1$, find an upper bound on R for any squeezing in terms of $|\tau|^2$.

(This exercise shows that loss reduces and limits the amount of squeezing.)

10.2. Optical parametric amplification (OPA)

The Hamiltonian given by Eq. (10.1) is what we need to squeeze a quadrature, but to learn how we can implement it in practice, first we have to discuss a little bit of **nonlinear optics** here.

10.2.1. Origin of nonlinearity. To model passive linear optics, Chapter 6 assumes that the matter modes are harmonic oscillators coupled to the EM modes, while Exercise 6.2 says that the resulting normal modes are hybrid EM-matter modes called polaritons. Optical nonlinearity comes from the fact that, if we have some special material, e.g., lithium niobate ($LiNbO_3$) or potassium titanyl phosphate (KTP), and the mode amplitudes are strong, e.g., when strong laser beams are used, the matter modes no longer behave as harmonic oscillators exactly and are more accurately modeled as **anharmonic oscillators**.

To correct for the anharmonicity, we add to the Hamiltonian a term $f(\hat{\boldsymbol{b}})$ that is **cubic** with respect to the matter-mode operators $\{\hat{b}_j\}$, i.e.,

$$\hat{H} = \hbar \sum_{j,l} F_{jl}\hat{c}_j^\dagger \hat{c}_l + f(\hat{\boldsymbol{b}}), \tag{10.20}$$

$$f(\hat{\boldsymbol{b}}) = \sum_{j,l,m} C_{jlm}\hat{b}_j\hat{b}_l\hat{b}_m + D_{jlm}\hat{b}_j^\dagger\hat{b}_l\hat{b}_m + \text{H.c.}, \tag{10.21}$$

where $\{C_{jlm}\}$ and $\{D_{jlm}\}$ are constants, the specific values of which are unimportant to our discussion. (We could add higher-than-cubic terms as well, but it's sufficient to stick with cubic here to model an OPA.) Rewrite

the Hamiltonian in terms of the polariton-mode operators $\{\hat{d}_j\}$ as per Exercise 6.2 by assuming $\hat{c}_j = \sum_l W_{jl}\hat{d}_l$. Then $\{\hat{b}_j\}$ can be expressed as linear functions of $\{\hat{d}_j\}$, and $f(\hat{\boldsymbol{b}})$ would become cubic with respect to $\{\hat{d}_j\}$, i.e., the Hamiltonian would look like

$$\hat{H} = \hbar\sum_j \omega_j \hat{d}_j^\dagger \hat{d}_j + g(\hat{\boldsymbol{d}}), \tag{10.22}$$

$$g(\hat{\boldsymbol{d}}) = \sum_{j,l,m} C'_{jlm}\hat{d}_j\hat{d}_l\hat{d}_m + D'_{jlm}\hat{d}_j^\dagger\hat{d}_l\hat{d}_m + \text{H.c.}, \tag{10.23}$$

where $g(\hat{\boldsymbol{d}})$ is cubic with respect to the $\hat{\boldsymbol{d}}$ operators and $\{C'_{jlm}\}$ and $\{D'_{jlm}\}$ are some other constants. In other words, the polariton modes no longer behave exactly as harmonic oscillators; they become anharmonic because they are partly matter modes.

For the sake of discussion, suppose that there are only two polariton modes: the first mode has a natural frequency $\omega_1 = \omega$ and the second mode has a natural frequency $\omega_2 = 2\omega$ that is **twice the frequency of the first mode (called second harmonic)**. The cubic term $g(\hat{\boldsymbol{d}})$ becomes

$$g(\hat{\boldsymbol{d}}) = C'_{111}\hat{d}_1^3 + C'_{112}\hat{d}_1^2\hat{d}_2 + \cdots + + D'_{211}\hat{d}_2^\dagger\hat{d}_1^2 + \text{H.c.}. \tag{10.24}$$

Now go to the interaction picture, assuming

$$\hat{H}_{\text{easy}} = \hbar\sum_j \omega_j \hat{d}_j^\dagger\hat{d}_j, \qquad\qquad \hat{\eta} = g(\hat{\boldsymbol{d}}). \tag{10.25}$$

Then we can replace $\hat{d}_j$ by $\hat{d}_j\exp(-i\omega_j t)$ in $g(\hat{\boldsymbol{d}})$ to compute the interaction-picture Hamiltonian $\hat{\eta}_{\text{easy}}(t)$. Eq. (10.24) becomes

$$\hat{\eta}_{\text{easy}}(t) = C'_{111}\hat{d}_1^3 e^{-3i\omega t} + C'_{112}\hat{d}_1^2\hat{d}_2 e^{-4i\omega t} + \cdots + D'_{211}\hat{d}_2^\dagger\hat{d}_1^2 + \text{H.c.}. \tag{10.26}$$

Of all the terms in $g(\hat{\boldsymbol{d}})$, notice that the last term $\propto \hat{d}_2^\dagger\hat{d}_1^2$ and its Hermitian conjugate $\propto \hat{d}_2\hat{d}_1^{\dagger 2}$ in Eq. (10.26) are special—**they stay constant in time while everything else oscillates at multiples of** ω. In the rotating-wave approximation (see Sec. D.5), we throw away all the terms in the Hamiltonian that oscillate quickly in time, because they average to zero over time and their net effect is negligible. We are left with

$$\hat{\eta}_{\text{easy}}(t) \approx D'_{211}\hat{d}_2^\dagger\hat{d}_1^2 + \text{H.c.}. \tag{10.27}$$

If we assume that the second mode has a strong amplitude and can be approximated as classical, then we can replace $\hat{d}_2$ by the complex amplitude α_2, and we are left with

$$\hat{\eta}_{\text{easy}}(t) \approx D'_{211}\alpha_2^*\hat{d}_1^2 + \text{H.c.}, \tag{10.28}$$

which explains the physical origin of the $\hat{a}^2$ and $\hat{a}^{\dagger 2}$ terms in Eq. (10.1).

It's helpful to think about what a Hamiltonian given by Eq. (10.27) does to a state for a tiny time step:

$$\exp\left(-\frac{i}{\hbar}\hat{\eta}_{\text{easy}}\Delta t\right)|\psi\rangle \approx \left(\hat{I} - \frac{i}{\hbar}\hat{\eta}_{\text{easy}}\Delta t\right)|\psi\rangle\,. \tag{10.29}$$

The term $\propto \hat{d}_2\hat{d}_1^{\dagger 2}$ in $\hat{\eta}_{\text{easy}}$ converts one second-harmonic polariton at 2ω to two polaritons at ω, while the term $\hat{d}_2^\dagger\hat{d}_1^2$ converts two polaritons at ω to one second-harmonic polariton at 2ω.

When light goes from free space into a crystal, the photons are converted to polaritons as they enter and polaritons are converted back to photons as they leave. The net effect of the crystal is to convert one second-harmonic photon to two lower-frequency photons (down conversion) or convert two photons into a second-harmonic photon (second-harmonic generation). The efficiency of each process depends on the experimental setup; please consult nonlinear optics textbooks, such as Refs. [15, 16, 17], for further details.

In practice, it'd be too tedious to go any further with this quantum approach. There are many other ways of deriving a quantum model of OPA and there's a lot more physics in OPA and nonlinear optics in general, but the most common approach, similar to how we dealt with passive linear optics in Chapter 6, is this:

(1) Derive the classical equations of motion using classical optics.

(2) Replace the c-number amplitudes by operators of some modes.
(3) Guess a Hermitian Hamiltonian such that the quantum equations of motion can be shown to arise from the Heisenberg picture. The Hermitian Hamiltonian ensures that we don't violate any fundamental principle of quantum mechanics.
(4) If we can't find a Hermitian Hamiltonian or something is wrong with the quantum equations of motion (e.g., it doesn't preserve the commutation relations), we'll have to fix it somehow; Chapter 7 is an example regarding loss.

10.2.2. Nonlinear optics. We now consult classical nonlinear optics to see how an OPA works in practice. Recall the usual model of EM fields in matter reviewed in Appendix F. When the polarization field $\boldsymbol{P}(\boldsymbol{r},t)$ is a function of the electric field $\boldsymbol{E}(\boldsymbol{r},t)$, the matter is called a dielectric. In most dielectrics we use in optics (crystals, glasses, plastics, semiconductors, etc.), the polarization field $\boldsymbol{P}(\boldsymbol{r},t)$ at each position $\boldsymbol{r}$ reacts only to the electric field $\boldsymbol{E}(\boldsymbol{r},t)$ at the same position $\boldsymbol{r}$ (we call this a local response). The time-domain behavior is slightly more complicated, but for our purpose in this section we can also assume that $\boldsymbol{P}(\boldsymbol{r},t)$ at each time reacts to the electric field at the same time t (we call this an instantaneous response). The precise dependence of $\boldsymbol{P}$ on $\boldsymbol{E}$ may still be complicated, but it is often sufficient to consider the Taylor expansion

$$P_j(\boldsymbol{r},t) = \underbrace{\epsilon_0 \sum_{l=x,y,z} \chi^{(1)}_{jl} E_l(\boldsymbol{r},t)}_{P^{(1)}_j} + \underbrace{\epsilon_0 \sum_{l,m} \chi^{(2)}_{jlm} E_l(\boldsymbol{r},t) E_m(\boldsymbol{r},t)}_{P^{(2)}_j} + \dots, \qquad j = x,y,z, \tag{10.30}$$

and keep the first few orders. $\chi^{(1)}$ and $\chi^{(2)}$ are called **optical susceptibility** tensors: $\chi^{(1)}$ is a tensor that maps a vector to a vector, while $\chi^{(2)}$ is a higher-order tensor that maps two vectors to one vector. The nice thing about this expression is that we no longer need to care about the matter degrees of freedom, as everything depends only on the electric field, and the role of the matter is modeled simply by the susceptibility tensors $\chi^{(1)}, \chi^{(2)}$, etc., that one can measure experimentally. For reasons that come from solid-state physics, $\chi^{(2)}$ is nonzero only for special crystals, such as lithium niobate ($LiNbO_3$) and potassium titanyl phosphate (KTP).

It can be shown that this classical picture is consistent with a quantum approach if we add a new term to the EM Hamiltonian [18]:

$$\hat{H} = \hat{H}_{\text{EM}} + \epsilon_0 \iiint \left[\frac{1}{2} \sum_{j,l} \chi^{(1)}_{jl} \hat{\boldsymbol{E}}_j(\boldsymbol{r}) \hat{\boldsymbol{E}}_l(\boldsymbol{r}) + \frac{2}{3} \sum_{j,l,m} \chi^{(2)}_{jlm} \hat{\boldsymbol{E}}_j(\boldsymbol{r}) \hat{\boldsymbol{E}}_l(\boldsymbol{r}) \hat{\boldsymbol{E}}_m(\boldsymbol{r}) + \dots \right] d^3\boldsymbol{r}, \tag{10.31}$$

where $\hat{\boldsymbol{E}}$ is expressed in terms of annihilation $\{\hat{a}_j\}$ and creation operators $\{\hat{a}_j^\dagger\}$ just as before.

Unlike the discussion in Sec. 10.2.1 based on the true physical origin of nonlinearity, Eq. (10.31) is derived by peeking at classical optics and guessing a Hamiltonian that is consistent with it [18]. To my knowledge, no one has bothered to explicitly derive Eq. (10.31) from first principles, although we can see that both approaches produce the same form of Hamiltonian, with quadratic and cubic terms with respect to the annihilation and creation operators.

If we keep only the $\chi^{(1)}$ term, the model is called a linear dielectric. We need the $\chi^{(2)}$ term as well to model an OPA. Suppose

$$\hat{H}_{\text{easy}} = \hat{H}_{\text{EM}} + \frac{\epsilon_0}{2} \iiint \sum_{j,l} \chi^{(1)}_{jl} \hat{\boldsymbol{E}}_j(\boldsymbol{r}) \hat{\boldsymbol{E}}_l(\boldsymbol{r}) d^3\boldsymbol{r}, \tag{10.32}$$

$$\hat{\eta} = \frac{2\epsilon_0}{3} \iiint \sum_{j,l,m} \chi^{(2)}_{jlm} \hat{\boldsymbol{E}}_j(\boldsymbol{r}) \hat{\boldsymbol{E}}_l(\boldsymbol{r}) \hat{\boldsymbol{E}}_m(\boldsymbol{r}) d^3\boldsymbol{r}. \tag{10.33}$$

Then we can regard $\hat{H}_{\text{easy}}$ as the simple Hamiltonian for the polaritons discussed in Chapter 6. We know from classical optics that the polaritons in a crystal are also sinusoidal plane waves, although the frequency $\omega(\boldsymbol{k},s)$ and the polarization $\tilde{\boldsymbol{e}}(\boldsymbol{k},s)$ of each mode is a bit different from the free-space case.

Let's go to the interaction picture. $\hat{\eta}_{\text{easy}}(t)$ would become a linear combination of many cubic terms with respect to $\{\hat{a}_j\}$ and $\{\hat{a}_j^\dagger\}$, although many of them can be thrown away through the rotating-wave approximation. More terms

can be thrown away if they turn out to be negligible after the $\iiint(\dots)d^3\boldsymbol{r}$ integral is performed. To understand how, recall that the electric field is a linear combination of $\exp(\pm i\boldsymbol{k}\cdot\boldsymbol{r})$ terms for the sinusoidal plane-wave modes. If we expand $\chi^{(2)}_{jlm}\hat{\boldsymbol{E}}_j(\boldsymbol{r})\hat{\boldsymbol{E}}_l(\boldsymbol{r})\hat{\boldsymbol{E}}_m(\boldsymbol{r})$, we find a lot of terms that oscillate in space, and they would become relatively small after the integration, while terms that stay constant in space become relatively large. For example, consider one "fundamental" mode with frequency ω and polarization $\tilde{\boldsymbol{e}}_1=\tilde{\boldsymbol{y}}$ and one "second-harmonic" mode with frequency 2ω and polarization $\tilde{\boldsymbol{e}}_2=\tilde{\boldsymbol{z}}$. Assume that both propagate in the $\tilde{\boldsymbol{x}}$ direction, as depicted in Fig. 10.2. The term in $\hat{\eta}_{\text{easy}}(t)$ that is relevant to the two modes looks like

$$\iiint \chi^{(2)}_{yyz}\hat{a}_2\hat{a}_1^{\dagger 2}\exp[i(k_2-2k_1)x]d^3\boldsymbol{r}+\text{H.c.}, \tag{10.34}$$

where k_1 is the wavenumber of the fundamental mode and k_2 is the wavenumber of the second-harmonic mode. The integration along the length L of the crystal would yield

$$\int_{-L/2}^{L/2}\exp[i(k_2-2k_1)x]dx=\begin{cases}L, & k_2-2k_1=0,\\ \dfrac{\sin[(k_2-2k_1)L/2]}{(k_2-2k_1)/2}, & k_2-2k_1\neq 0.\end{cases} \tag{10.35}$$

If $k_2-2k_1=0$, then we say that the **phase-matching condition** is satisfied and the integral would grow with L, but if $k_2-2k_1\neq 0$, then the integral does not grow with L and is inversely proportional to the mismatch k_2-2k_1.

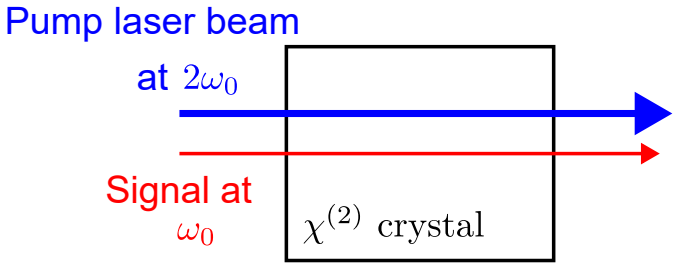

FIGURE 10.2. An optical parametric amplifier. (The pump beam and the signal beam are actually overlapping optical beams in practice, and a dichroic mirror (https://www.rp-photonics.com/dichroic_mirrors.html) is used to combine or separate the two beams.)

Side note. *I have assumed a Cartesian coordinate system that is aligned with the principal axes of a KTP crystal, the most commonly used crystal in optical squeezing.* $\chi^{(2)}_{yyz}$ *happens to be nonzero in a KTP crystal, so the propagation direction is chosen to be the* $\tilde{\boldsymbol{x}}$ *axis.*

In a crystal, usually $k_2-2k_1\neq 0$, but a technique called **quasi-phase matching** can be used to compensate for the mismatch (https://en.wikipedia.org/wiki/Quasi-phase-matching). The idea is to apply "periodic polling" to the crystal through high voltages, so that the domains of the crystal are periodically switched and $\chi^{(2)}(x)$ switches sign periodically along x. Now we can write $\chi^{(2)}$ as the Fourier series

$$\chi^{(2)}(x)=C\exp\left(i\frac{2\pi}{\Lambda}x\right)+\text{c.c.}+\dots, \tag{10.36}$$

where C is the Fourier coefficient and Λ is the period of the polling. If

$$\frac{2\pi}{\Lambda}=|k_2-2k_1|, \tag{10.37}$$

the $\exp(\pm i2\pi x/\Lambda)$ terms in $\chi^{(2)}$ can cancel the $\exp[\pm i(k_2-2k_1)x]$ terms, $\chi^{(2)}(x)\exp[i(k_2-2k_1)x]$ then contains a constant term, and after the $\int_{-L/2}^{L/2}(\dots)dx$ integration, the constant term becomes $\propto L$ that grows with the crystal length L.

With phase matching and a strong "pump" laser beam at 2ω with $\hat{a}_2 \approx \alpha_2$, it is possible to simplify $\hat{\eta}_{\text{easy}}(t)$ to

$$\hat{\eta}_{\text{easy}}(t) \propto \alpha_2 \hat{a}_1^{\dagger 2} + \text{H.c.}, \tag{10.38}$$

where all other terms are thrown away because of either the rotating-wave approximation or phase mismatch. This result now agrees with Eq. (10.1) that we assumed earlier.

Notice that the ξ parameter in Eq. (10.1) is proportional to the amplitude α_2 of the pump, so we can choose the squeezed and antisqueezed quadratures by changing the phase of the pump.

Side note. *To enhance the squeezing, the crystal is often put inside an optical cavity so that the signal optical beam passes through the crystal many times [9]. While a more complicated model is needed [19] to model the setup and the multimode squeezing that comes out of it, the single-mode model here captures the essential physics and is good enough for an undergraduate corse.*

Side note. *The word "parametric" comes from the fact that, when there is a strong laser pump beam at frequency $2\omega_0$, we can also model the OPA by assuming that the "parameter" of the system $\chi^{(1)}$ oscillates at frequency $2\omega_0$. Historically, parametric interactions have been studied since Faraday and Rayleigh (https://en.wikipedia.org/wiki/Parametric_oscillator). A textbook example is a child "pumping" a swing at twice the natural frequency of the swing, where the moment of inertia is the "parameter" to be modulated in time. With radio/microwave circuits, it's also possible to see the same parametric amplification behavior by modulating the capacitance or inductance at twice the frequency of a signal to be amplified.*

10.3. Squeezed vacuum state

Let's return to the formalism in Sec. 10.1 and study more general properties of squeezing. Define a **squeeze operator** as

$$\boxed{\hat{S}(z) \equiv \exp\left(\frac{1}{2} z \hat{a}^{\dagger 2} - \text{H.c.}\right),} \qquad z \in \mathbb{C}. \tag{10.39}$$

Convince yourself that this is the unitary operator resulting from the Hamiltonian given by Eq. (10.1), with

$$z = \xi t. \tag{10.40}$$

It follows from Sec. 10.1 that the Heisenberg picture of $\hat{a}$ under this unitary is given by

$$\boxed{\hat{S}^\dagger(z) \hat{a} S(z) = \hat{a} \cosh|z| + e^{i\angle z} \hat{a}^\dagger \sinh|z|.} \tag{10.41}$$

Now imagine that we measure a quadrature

$$\hat{q}(\theta) \equiv \frac{1}{\sqrt{2}} \left(e^{-i\theta} \hat{a} + e^{i\theta} \hat{a}^\dagger\right) \tag{10.42}$$

after squeezing the vacuum (see Exercise 4.26 for basic properties of $\hat{q}(\theta)$). The probability density of the outcome is given by

$$f(x) = |\langle q(\theta) = x| \hat{S}(z) |0\rangle|^2 = \langle 0| \hat{S}^\dagger(z) |q(\theta) = x\rangle \langle q(\theta) = x| \hat{S}(z) |0\rangle, \tag{10.43}$$

where $\hat{S}(z)|0\rangle$ is called a **squeezed vacuum state**. To compute this, we take the following steps:

(1) Define the Heisenberg picture of $\hat{q}(\theta)$ as

$$\hat{O} \equiv \hat{S}^\dagger(z) \hat{q}(\theta) \hat{S}(z). \tag{10.44}$$

It allows us to write the diagonal form of $\hat{O}$ in two ways:

$$\hat{O} = \int_{-\infty}^{\infty} x |O = x\rangle \langle O = x| dx = \hat{S}^\dagger(z) \hat{q}(\theta) \hat{S}(z) = \int_{-\infty}^{\infty} x \hat{S}^\dagger(z) |q(\theta) = x\rangle \langle q(\theta) = x| \hat{S}(z) dx. \tag{10.45}$$

A nontrivial theorem in Hilbert-space theory [20, Theorem VIII.6] says that the diagonal form is unique, so that we can write

$$\hat{S}^\dagger(z)\,|q(\theta)=x\rangle\,\langle q(\theta)=x|\,\hat{S}(z) = |O=x\rangle\,\langle O=x|\,. \tag{10.46}$$

Now we need to find $|O=x\rangle$.

(2) Use Eq. (10.41) to obtain

$$\hat{O} = \frac{1}{\sqrt{2}}\left(g^*\hat{a} + g\hat{a}^\dagger\right), \qquad \boxed{g \equiv e^{i\theta}\cosh|z| + e^{-i\theta}e^{i\angle z}\sinh|z|.} \tag{10.47}$$

(3) Rewrite $\hat{O}$ in terms of another quadrature operator:

$$\hat{O} = |g|\frac{1}{\sqrt{2}}\left(e^{-i\angle g}\hat{a} + e^{i\angle g}\hat{a}^\dagger\right) = |g|\hat{q}(\angle g), \tag{10.48}$$

$$\hat{q}(\angle g) \equiv \frac{1}{\sqrt{2}}\left(e^{-i\angle g}\hat{a} + e^{i\angle g}\hat{a}^\dagger\right). \tag{10.49}$$

$|g|$ determines how much the quadrature is amplified or squeezed. Exercise D.6 shows that, given Eq. (10.48), the orthonormal eigenstates of $\hat{O}$ can be expressed in terms of the orthonormal eigenstates of $\hat{q}(\angle g)$ as

$$|O=x\rangle = \frac{1}{\sqrt{|g|}}\left|q(\angle g) = \frac{x}{|g|}\right\rangle. \tag{10.50}$$

(4) Now we can rewrite Eq. (10.43) as

$$\begin{aligned}
f(x) &= \langle 0|\,\hat{S}^\dagger(z)\,|q(\theta)=x\rangle\,\langle q(\theta)=x|\,\hat{S}(z)\,|0\rangle && && (10.51)\\
&= \langle 0|O=x\rangle\,\langle O=x|0\rangle && \text{(using Eq. (10.46))} && (10.52)\\
&= |\langle O=x|0\rangle|^2 && && (10.53)\\
&= \frac{1}{|g|}\left|\left\langle q(\angle g) = \frac{x}{|g|}\middle|0\right\rangle\right|^2 && \text{(using Eq. (10.50))} && (10.54)\\
&= \boxed{\frac{1}{\sqrt{\pi}|g|}\exp\left(-\frac{x^2}{|g|^2}\right).} && \text{(using Exercise 4.26)} && (10.55)
\end{aligned}$$

This is a new result, showing that **any quadrature of a squeezed vacuum state is Gaussian with zero mean and a variance given by** $|g|^2/2$, where the g parameter is given by Eq. (10.47). The variance depends on the quadrature being measured through the θ parameter and the phase of the pump through the $\angle z$ parameter. For example, if we set

$$\theta = \frac{1}{2}\angle z, \qquad g = e^{i(\angle z)/2}e^{|z|}, \qquad \frac{|g|^2}{2} = \frac{1}{2}e^{2|z|}, \tag{10.56}$$

then the variance of $\hat{q}(\theta)$ is $|g|^2/2 = e^{2|z|}/2$, which agrees with Eq. (10.15) that we derived earlier for the antisqueezed quadrature using the Heisenberg picture. On the other hand, if we set

$$\theta = \frac{\pi}{2} + \frac{1}{2}\angle z, \qquad g = ie^{i(\angle z)/2}e^{-|z|}, \qquad \frac{|g|^2}{2} = \frac{1}{2}e^{-2|z|}, \tag{10.57}$$

then the variance agrees with Eq. (10.16) for the squeezed quadrature.

We have found so far that both the coherent states and the squeezed vacuum states have Gaussian probability densities for any of their quadratures. It turns out that they are special examples of a general class of states called **Gaussian states**, defined by the property that any quadrature of such a state has a Gaussian probability density. Gaussian states are important states for quantum optics and quantum information, because Gaussian states are relatively easy to generate, it can be shown that they remain Gaussian states after going through passive linear optics and squeezing, and they give Gaussian probability densities for homodyne and heterodyne detection. Chapter 11

will introduce a theoretical concept called the Wigner representation that will be very handy for studying and visualizing Gaussian states.

Exercise 10.7. Derive the probability density

$$\left|\langle q(\theta) = x|\, \hat{S}(z)\, |\alpha\rangle\right|^2 \tag{10.58}$$

of a quadrature for a squeezed coherent state $\hat{S}(z)\,|\alpha\rangle$.

CHAPTER 11

Wigner Representation

11.1. Definition

The Wigner representation of a quantum state is similar to the Sudarshan representation and useful for a lot of calculations, as well as visualization of a quantum state. To introduce it, we first focus on just one optical mode and introduce a preliminary concept called the **quantum characteristic function**. It is defined as

$$\boxed{\chi(\xi,\eta) \equiv \mathrm{tr}\left[\hat{\rho}\exp(i\xi\hat{q}+i\eta\hat{p})\right],} \qquad (\xi,\eta)\in\mathbb{R}^2, \tag{11.1}$$

where (ξ,η) are two real variables. This is a generalization of the characteristic function in probability theory (https://en.wikipedia.org/wiki/Characteristic_function_(probability_theory)). If $f_{XY}(x,y)$ is the joint probability density for two real random variables X and Y, the classical characteristic function is defined as

$$\chi_{\text{classical}}(\xi,\eta) \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_{XY}(x,y)\exp(i\xi x+i\eta y)dxdy = \mathbb{E}\left[\exp(i\xi X+i\eta Y)\right], \tag{11.2}$$

except that the quantum version replaces the random variables X and Y by the quadrature operators $\hat{q}$ and $\hat{p}$. In the classical case, the probability density $f_{XY}(x,y)$ can be obtained from $\chi_{\text{classical}}(\xi,\eta)$ because of the Fourier-transform relations:

$$f_{XY}(x,y) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\chi_{\text{classical}}(\xi,\eta)\exp(-i\xi x-i\eta y)d\xi d\eta. \tag{11.3}$$

In the quantum case, the Wigner representation is defined similarly in terms of the quantum χ:

$$\boxed{W(x,y) \equiv \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\chi(\xi,\eta)\exp(-i\xi x-i\eta y)d\xi d\eta.} \tag{11.4}$$

The Wigner representation is a function of two real variables (x,y) called the **phase-space variables** and it often behaves like a joint probability density of the two quadratures $\hat{q}$ and $\hat{p}$, but do note that it can go **negative** for some (x,y) for certain states. Since it may go negative, the Wigner representation is also sometimes called the Wigner quasiprobability distribution.

Exercise 11.1. An alternative definition of the Wigner representation is

$$W(x,y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\lambda y}\left\langle q=x-\frac{\lambda}{2}\right|\hat{\rho}\left|q=x+\frac{\lambda}{2}\right\rangle d\lambda. \tag{11.5}$$

Show that this definition is equivalent to Eq. (11.4).

11.2. Probability densities of quadratures

The Wigner representation is useful mainly because it is easy to compute **the probability density of any quadrature** from it. In particular, it can be shown that, for any state,

$$\boxed{\langle q=x|\,\hat{\rho}\,|q=x\rangle = \int_{-\infty}^{\infty}W(x,y)dy,} \qquad \boxed{\langle p=y|\,\hat{\rho}\,|p=y\rangle = \int_{-\infty}^{\infty}W(x,y)dx,} \tag{11.6}$$

so the **marginal densities** computed from the Wigner representation are the probability densities of the $\hat{q}$ and $\hat{p}$ quadratures. In this way $W(x,y)$ behaves like the joint probability density of the two quadratures.

More generally, if we define rotated quadratures

$$\hat{q}(\theta) \equiv \hat{q}\cos\theta + \hat{p}\sin\theta = \frac{1}{\sqrt{2}}\left(e^{-i\theta}\hat{a} + e^{i\theta}\hat{a}^\dagger\right), \tag{11.7}$$

$$\hat{p}(\theta) \equiv -\hat{q}\sin\theta + \hat{p}\cos\theta = \frac{1}{\sqrt{2}i}\left(e^{-i\theta}\hat{a} - e^{i\theta}\hat{a}^\dagger\right), \tag{11.8}$$

then the Wigner representation can also give their probability distributions as follows:

(1) Define

$$u(x,y) = x\cos\theta + y\sin\theta, \qquad v(x,y) = -x\sin\theta + y\cos\theta, \tag{11.9}$$

which are the phase-space coordinates for the new quadratures given by Eqs. (11.7) and (11.8). The new phase-space coordinate system is shown in Fig. 11.1. The inverse relations are

$$x(u,v) = u\cos\theta - v\sin\theta, \qquad y(u,v) = u\sin\theta + v\cos\theta. \tag{11.10}$$

(2) Define a new Wigner representation $W'(u,v)$ as

$$W'(u,v) \equiv W(x(u,v), y(u,v)). \tag{11.11}$$

(3) The marginal distributions with respect to the new W' turn out to be the probability distributions of $\hat{q}(\theta)$ and $\hat{p}(\theta)$:

$$\boxed{\langle q(\theta) = u|\,\hat{\rho}\,|q(\theta) = u\rangle = \int_{-\infty}^{\infty} W'(u,v)dv,} \qquad \boxed{\langle p(\theta) = v|\,\hat{\rho}\,|p(\theta) = v\rangle = \int_{-\infty}^{\infty} W'(u,v)du.} \tag{11.12}$$

(This property for any quadrature is why the Wigner representation is much more useful than just multiplying $\langle q = x|\,\hat{\rho}\,|q = x\rangle$ and $\langle p = y|\,\hat{\rho}\,|p = y\rangle$ together.)

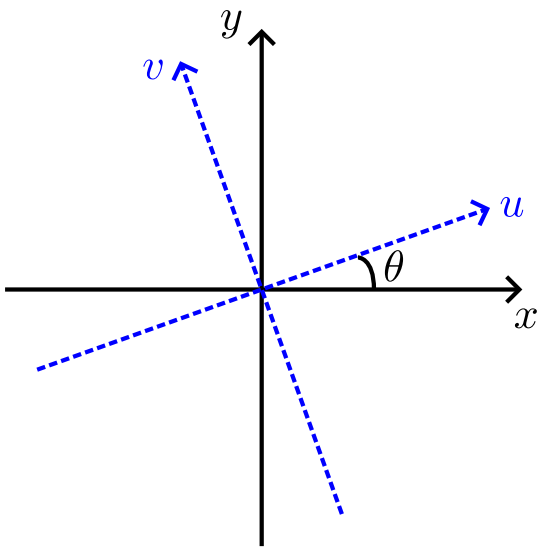

FIGURE 11.1. The new phase-space coordinate system defined by Eqs. (11.9).

This procedure of computing the new Wigner representation is exactly the same as the procedure of computing a new probability density $f_{UV}(u,v)$ from $f_{XY}(x,y)$ if the new random variables are related to the old ones by

$$U = X\cos\theta + Y\sin\theta, \qquad V = -X\sin\theta + Y\cos\theta. \tag{11.13}$$

The Wigner representation behaves like a joint probability density of quadratures in this way. Do note, however, the following key caveats:

(1) For certain states, $W(x,y)$ **may go negative** for some phase-space coordinates (x,y), so it cannot always be regarded as a probability density.

(2) $W(x,y)$ by itself is not the probability density of any measurement. It gives the probability density of a quadrature measurement only after we compute the **marginal** as per Eqs. (11.6) or Eqs. (11.12).
(3) It is not so easy to compute from $W(x,y)$ the probability distributions for measurements other than quadrature measurements, so it's not nearly as useful for other measurements.

Exercise 11.2. Derive Eqs. (11.6).

Exercise 11.3. Prove that the Wigner representation is normalized as

$$\boxed{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(x,y)dxdy = 1.} \tag{11.14}$$

Exercise 11.4. Derive Eqs. (11.12).

Exercise 11.5. Let $W(x,y)$ be the Wigner representation of $\hat{\rho}$. Find the Wigner representations of the following density operators in terms of $W(x,y)$:

(1) $\hat{D}(\alpha)\hat{\rho}\hat{D}^\dagger(\alpha)$, where $\hat{D}(\alpha)$ is the displacement operator.
(2) $\hat{R}(\theta)\hat{\rho}\hat{R}^\dagger(\theta)$, where $\hat{R}(\theta)$ is the "rotation" operator defined by Eq. (4.53).
(3) $\hat{S}(z)\hat{\rho}\hat{S}^\dagger(z)$, where $\hat{S}(z)$ is the squeeze operator defined by Eq. (10.39).

(This exercise shows that, if the unitary operator for the dynamics can be decomposed into a product of these three operators, then the Wigner representation in the Schrödinger picture is easy to find.)

11.3. Examples

11.3.1. Coherent state. It is easy to show that, for a coherent state,

$$\boxed{\hat{\rho} = |\alpha\rangle\langle\alpha| : \quad W(x,y) = \frac{1}{\pi}\exp\left[-\left(x-\sqrt{2}\,\mathrm{Re}\,\alpha\right)^2 - \left(y-\sqrt{2}\,\mathrm{Im}\,\alpha\right)^2\right].} \tag{11.15}$$

A plot of this Wigner representation in phase space is shown in Fig. 11.2. It coincides with a **Gaussian** probability density for two independent Gaussian random variables, each with variance $1/2$. This result agrees with the distributions $|\langle q = x|\alpha\rangle|^2$ and $|\langle p = y|\alpha\rangle|^2$ given by Eqs. (4.7) and (4.8). It also agrees with the distribution $|\langle q(\theta) = u|\alpha\rangle|^2$ that we computed in Exercise 4.26.

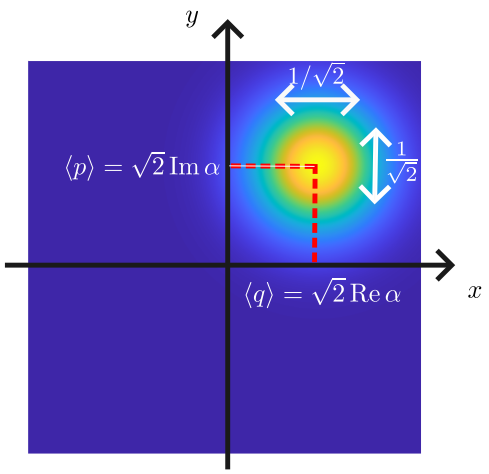

FIGURE 11.2. The Wigner representation of a coherent state in phase space.

Exercise 11.6. Derive Eq. (11.15).

11.3.2. Squeezed vacuum. For a squeezed vacuum state discussed in Chapter 10, it is easier to write the Wigner representation in terms of the new variables

$$u(x,y) = x\cos\frac{\angle z}{2} + y\sin\frac{\angle z}{2}, \qquad v(x,y) = -x\sin\frac{\angle z}{2} + y\cos\frac{\angle z}{2}, \tag{11.16}$$

so that

$$\boxed{\hat{\rho} = \hat{S}(z)\,|0\rangle\,\langle 0|\,\hat{S}^\dagger(z): \quad W(x,y) = W'(u,v) = \frac{1}{\pi}\exp\left(-\frac{u^2}{e^{2|z|}} - \frac{v^2}{e^{-2|z|}}\right).} \tag{11.17}$$

This result coincides with the probability density of two independent zero-mean Gaussian random variables U and V, where U has a variance $e^{2|z|}/2$ and V has a variance $e^{-2|z|}/2$, as depicted in Fig. 11.3. The new quadratures $\hat{q}(\frac{\angle z}{2})$ and $\hat{p}(\frac{\angle z}{2})$ coincide with the antisqueezed quadrature and squeezed quadrature, respectively, and it can be shown that this Wigner representation leads to a Gaussian probability density for any quadrature, in agreement with Sec. 10.3.

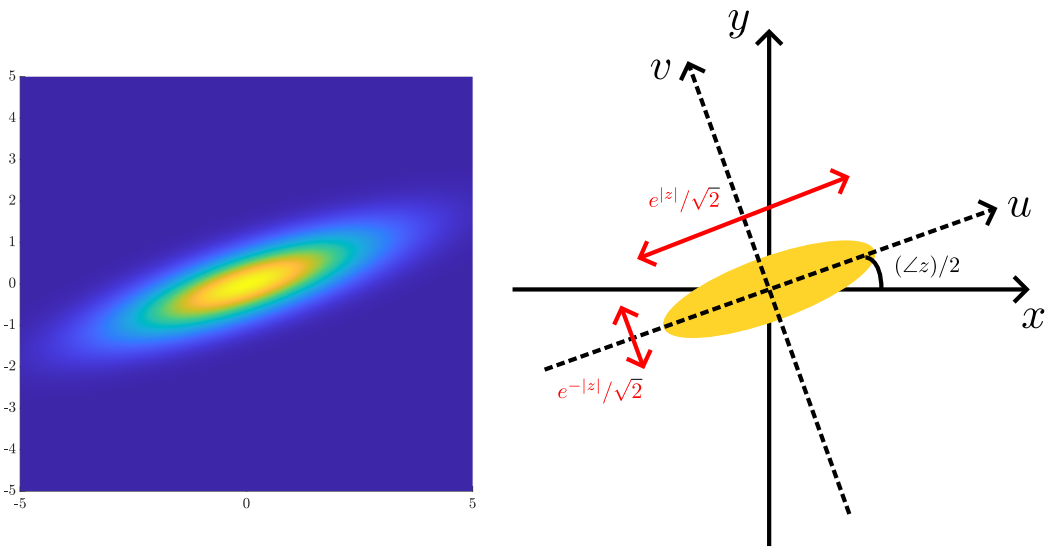

FIGURE 11.3. The Wigner representation of a squeezed vacuum state in phase space. This picture shows why we call it a squeezed state.

Notice that the Wigner representation remains nonnegative for the squeezed vacuum. The Sudarshan representation, on the other hand, cannot stay nonnegative for this state, as implied by Exercise 9.8.

Exercise 11.7. Derive Eq. (11.17).

11.3.3. Gaussian states. The coherent state and the squeezed vacuum state are examples of a larger class of states called the Gaussian states, which are defined as states with Gaussian Wigner representations:

$$W(x,y) = \frac{1}{2\pi\sqrt{\det\Sigma}}\exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{m})^\top\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{m})\right], \qquad \boldsymbol{x} \equiv \begin{pmatrix} x \\ y \end{pmatrix}. \tag{11.18}$$

While the mean vector $\boldsymbol{m}$ can be arbitrary, the covariance matrix Σ must satisfy the Heisenberg uncertainty relations for any two quadratures for $W(x,y)$ to be the Wigner representation of a legal quantum state.

The general theory of Gaussian states for multiple modes goes very deep; it is an active research topic in quantum information theory [21].

11.3.4. Number states. For $\hat{\rho} = |n\rangle\langle n|$, it's easier to use Eq. (11.5). Using also Eq. (4.1), we obtain

$$W(x,y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{i\lambda y}}{2^n n!\pi^{1/2}} H_n(x-\lambda/2)\exp\left[-\frac{(x-\lambda/2)^2}{2}\right] H_n(x+\lambda/2)\exp\left[-\frac{(x+\lambda/2)^2}{2}\right] d\lambda \quad (11.19)$$

$$= \frac{e^{-x^2}}{2\pi 2^n n!\pi^{1/2}}\int_{-\infty}^{\infty} e^{i\lambda y} H_n(x-\lambda/2)H_n(x+\lambda/2)\exp\left(-\frac{\lambda^2}{4}\right) d\lambda \quad (11.20)$$

$$= \frac{(-1)^n}{\pi} L_n[2(x^2+y^2)]e^{-x^2-y^2}, \quad (11.21)$$

where $L_n(u)$ is the nth Laguerre polynomial (https://en.wikipedia.org/wiki/Laguerre_polynomials). (I have to admit that I just copied the result from https://en.wikipedia.org/wiki/Wigner_quasiprobability_distribution#Examples.) For $n = 1$ in particular,

$$H_1(x-\lambda/2) = 2x - \lambda, \quad (11.22)$$

$$W(x,y) = \frac{e^{-x^2}}{(2\pi 2)\pi^{1/2}}\int_{-\infty}^{\infty} e^{i\lambda y}(4x^2-\lambda^2)\exp\left(-\frac{\lambda^2}{4}\right) d\lambda \quad (11.23)$$

$$= \frac{1}{\pi}(2x^2+2y^2-1)e^{-x^2-y^2}. \quad (11.24)$$

This function is plotted in Fig. 11.4. Notice that it goes **negative** in the middle of phase space, so we can't treat the Wigner representation here as a probability density. In general, $W(x,y)$ always goes negative somewhere in phase space for a number state with $n \geq 1$.

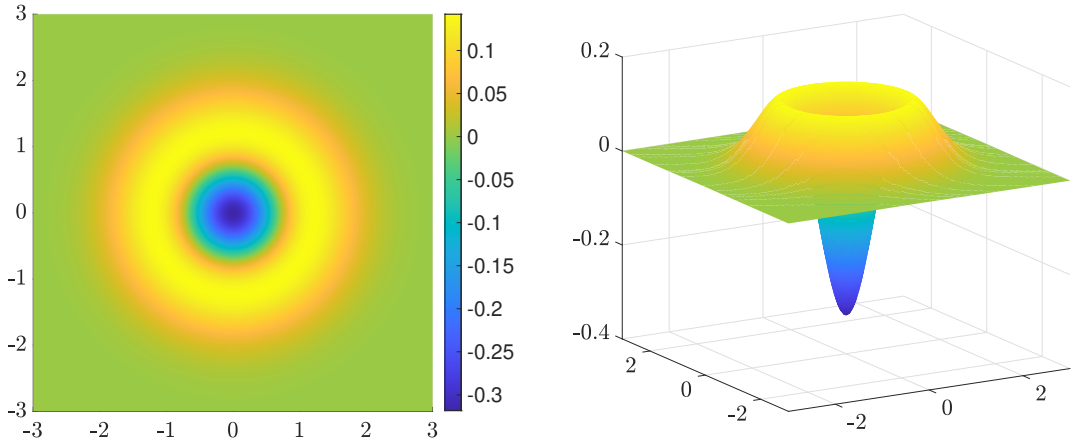

FIGURE 11.4. Wigner representation of the number state $|n\rangle$, $n = 1$.

The negativity of the Wigner representation is often regarded as another signature of nonclassicality for a quantum state. This criterion is a bit more stringent than the negativity of the Sudarshan representation, since there exist states with positive $W(x,y)$ for all (x,y), such as the squeezed vacuum state, but their Sudarshan representations can go negative.

11.4. Relations with other phase-space distributions

We have encountered three phase-space distributions so far:

(1) The Sudarshan representation $\Phi(\alpha)$ (Sec. 4.5).
(2) The Wigner representation $W(x,y)$.
(3) The so-called **Husimi** representation, also called the Q function:

$$\boxed{Q(\alpha) \equiv \frac{1}{\pi}\langle\alpha|\hat{\rho}|\alpha\rangle,} \quad (11.25)$$

which is precisely the probability density from dual-homodyne detection or heterodyne detection, as we found in Chapter 8.

It turns out that the three representations have a cute relationship. To show it, we first rewrite $W(x,y)$ in terms of a complex variable α:

$$\tilde{W}(\alpha) \equiv 2W(\sqrt{2}\,\mathrm{Re}\,\alpha, \sqrt{2}\,\mathrm{Im}\,\alpha), \qquad W(x,y) = \frac{1}{2}\tilde{W}\left(\frac{x+iy}{\sqrt{2}}\right). \tag{11.26}$$

The factor of 2 ensures that $\tilde{W}(\alpha)$ is normalized as

$$\iint \tilde{W}(\alpha) d^2\alpha = 1, \tag{11.27}$$

just like $\Phi(\alpha)$ and $Q(\alpha)$. The relations among the three are

$$\boxed{\tilde{W}(\alpha) = \iint \Phi(\beta) \frac{2}{\pi} \exp\left(-2|\alpha-\beta|^2\right) d^2\beta,} \tag{11.28}$$

$$\boxed{Q(\alpha) = \iint \Phi(\beta) \frac{1}{\pi} \exp\left(-|\alpha-\beta|^2\right) d^2\beta = \iint \tilde{W}(\beta) \frac{2}{\pi} \exp\left(-2|\alpha-\beta|^2\right) d^2\beta.} \tag{11.29}$$

Another way of writing these relations is in terms of the **convolution** $*$ between two functions (https://en.wikipedia.org/wiki/Convolution):

$$f * g \equiv \iint f(\beta) g(\alpha-\beta) d^2\beta, \tag{11.30}$$

$$\tilde{W} = \Phi * \left(\frac{2}{\pi} e^{-2|\alpha|^2}\right), \tag{11.31}$$

$$Q = \Phi * \left(\frac{1}{\pi} e^{-|\alpha|^2}\right) = W * \left(\frac{2}{\pi} e^{-2|\alpha|^2}\right). \tag{11.32}$$

The effect of convolution with a Gaussian function is like **diffusion**: it **blurs** the function in phase space. The simplest example is a coherent state $|\beta\rangle$:

$$\Phi(\alpha) = \delta^2(\alpha-\beta) \equiv \delta(\mathrm{Re}\,\alpha - \mathrm{Re}\,\beta)\delta(\mathrm{Im}\,\alpha - \mathrm{Im}\,\beta), \tag{11.33}$$

$$\tilde{W}(\alpha) = \frac{2}{\pi} \exp\left(-2|\alpha-\beta|^2\right), \tag{11.34}$$

$$Q(\alpha) = \frac{1}{\pi} \exp\left(-|\alpha-\beta|^2\right). \tag{11.35}$$

The first column of Figure 11.5 plots $\tilde{W}(\alpha)$ and $Q(\alpha)$ for a coherent state, the second column plots those of a squeezed vacuum state, while the third column plots $\tilde{W}(\alpha)$ and $Q(\alpha)$ for a number state $|n=1\rangle$. It's a lot more difficult to plot the Sudarshan representations for these common states, and the Wigner representation is the default phase-space distribution for plotting.

Exercise 11.8. Derive Eqs. (11.28) and (11.29).

Exercise 11.9. Consider a squeezed vacuum state with $\angle z = 0$. Compute the Husimi representation $Q(\alpha)$. Find the variances of the two quadratures in dual-homodyne detection. Using this result, explain why dual-homodyne detection is not used in interferometry with a squeezed state.

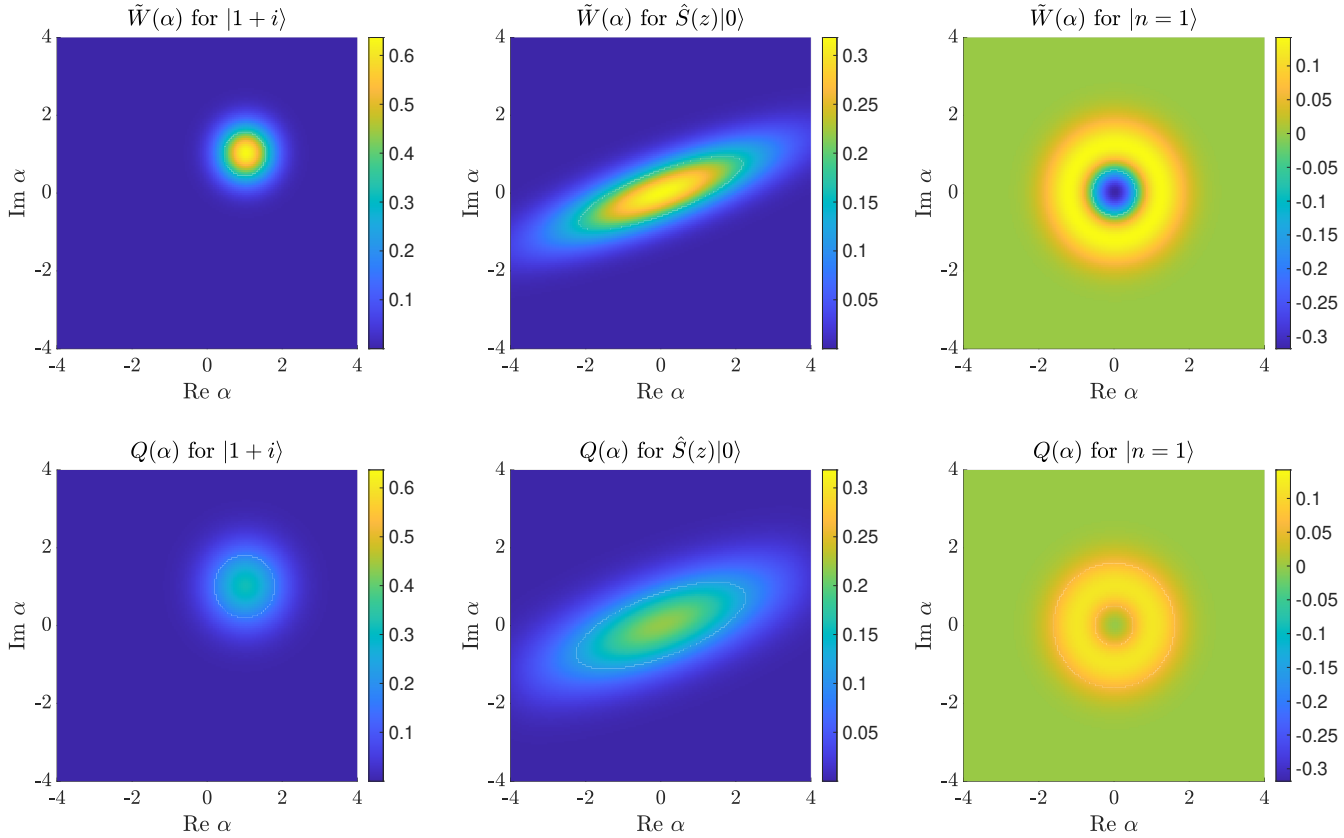

FIGURE 11.5. First column: Wigner $\tilde{W}(\alpha)$ and Husimi $Q(\alpha)$ for a coherent state $|1+i\rangle$. Second column: $\tilde{W}$ and Q for a squeezed vacuum state. Third column: $\tilde{W}$ and Q for a number state $|n=1\rangle$.

11.5. Multimode Wigner representation

Assume J modes. The quantum characteristic function and the Wigner representation are now defined as

$$\boxed{\chi(\boldsymbol{\xi},\boldsymbol{\eta}) \equiv \mathrm{tr}\,[\hat{\rho}\exp(i\boldsymbol{\xi}\cdot\hat{\boldsymbol{q}}+i\boldsymbol{\eta}\cdot\hat{\boldsymbol{p}})],} \tag{11.36}$$

$$\boldsymbol{\xi}\cdot\hat{\boldsymbol{q}}+\boldsymbol{\eta}\cdot\hat{\boldsymbol{p}} = \sum_j (\xi_j\hat{q}_j+\eta_j\hat{p}_j), \tag{11.37}$$

$$\boxed{W(\boldsymbol{x},\boldsymbol{y}) \equiv \frac{1}{(2\pi)^{2J}}\int \chi(\boldsymbol{\xi},\boldsymbol{\eta})\exp(-i\boldsymbol{\xi}\cdot\boldsymbol{x}-i\boldsymbol{\eta}\cdot\boldsymbol{y})d^J\boldsymbol{\xi}d^J\boldsymbol{\eta},} \tag{11.38}$$

$$\boldsymbol{\xi}\cdot\boldsymbol{x}+\boldsymbol{\eta}\cdot\boldsymbol{y} = \sum_j (\xi_j x_j+\eta_j y_j). \tag{11.39}$$

Exercise 11.10. Find $W(\boldsymbol{x},\boldsymbol{y})$ for a multimode coherent state $|\boldsymbol{\alpha}\rangle$.

CHAPTER 12

Spontaneous Parametric Down Conversion (SPDC)

12.1. Entangled photons

We now discuss another application of optical parametric amplifiers (OPA): generation of entangled photons. Entangled photons are useful for experiments in quantum foundations and quantum information.

I will give a quick overview of the optics involved, focusing on the experimental setup reported in Ref. [22]; see Fig. 12.1. This setup has been adopted in many other experiments; see, e.g., Refs. [23, 24].

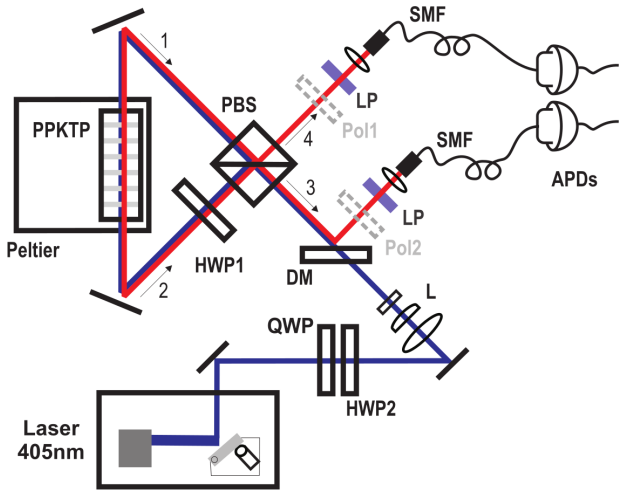

FIGURE 12.1. Experimental setup for generating entangled photons reported in Ref. [22] (Figure copied from Fig. 3 of the paper). PPKTP means "periodically poled KTP."

In the setup depicted in Fig. 12.1, there are two pump beams going into the crystal in counter-propagating directions, but let's focus on the physics with just one pump beam for now. Recall our discussion in Sec. 10.2.2, but now assume that there are three modes all propagating in the $+\tilde{\boldsymbol{x}}$ direction, with annihilation operators $\hat{a}_1$, $\hat{a}_2$, $\hat{a}_3$, respectively. Suppose that

(1) $\hat{a}_1$ is the annihilation operator of a **signal** mode with center frequency ω_0 and polarization vector $\tilde{\boldsymbol{e}}_1 = \tilde{\boldsymbol{y}}$.
(2) $\hat{a}_2$ is the annihilation operator of a so-called **idler** mode, which has the same properties as the signal mode except that the polarization vector is $\tilde{\boldsymbol{e}}_2 = \tilde{\boldsymbol{z}}$.
(3) $\hat{a}_3$ is the second-harmonic mode with frequency $2\omega_0$ and polarization vector $\tilde{\boldsymbol{e}}_3 = \tilde{\boldsymbol{y}}$.

Then the term in $\hat{\eta}_{\text{easy}}(t)$ relevant to the three modes would look like

$$\iiint \chi^{(2)}_{yzy}(x)\hat{a}_3\hat{a}_1^\dagger\hat{a}_2^\dagger \exp[i(k_3 - k_1 - k_2)x]d^3\boldsymbol{r} + \text{H.c.}, \tag{12.1}$$

where k_j is the wavenumber for mode j. If the crystal is periodically poled such that $\chi^{(2)}(x)$ compensates for the phase mismatch $k_3 - k_1 - k_2$, then this term would be enhanced over all other terms. Further, assume that the second-harmonic mode comes from a strong pump laser beam, such that $\hat{a}_3 \approx \alpha_3$. The interaction-picture

Hamiltonian becomes

$$\boxed{\hat{\eta}_{\text{easy}}(t) \approx g\alpha_3 \hat{a}_1^\dagger \hat{a}_2^\dagger + \text{H.c.},} \tag{12.2}$$

where g is a constant depending on $\chi^{(2)}$ and the length of the crystal.

Unlike the squeezing setup in Chapter 10, where we have just one signal mode at the fundamental frequency ω_0 and the Hamiltonian is proportional to $\hat{a}^2$ and $\hat{a}^{\dagger 2}$, here we have two modes at ω_0 called the signal and the idler with two different polarizations. The former case is called degenerate OPA and the latter case, with two different modes at the fundamental frequency, is called nondegenerate OPA. Since $k_1 \neq k_2$, $k_3 - k_1 - k_2$ is different from $k_3 - 2k_1$, and the efficiency of each process can be controlled by choosing the period of the poling to achieve quasi-phase matching for the desired process.

We now proceed with the first-order perturbation theory to obtain the interaction-picture quantum state:

$$|\psi_I(t)\rangle = \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau\right] \approx |\text{vac}\rangle - \frac{i}{\hbar}\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau\,|\text{vac}\rangle = |\text{vac}\rangle - \frac{ig\alpha_3}{\hbar}\hat{a}_1^\dagger\hat{a}_2^\dagger\,|\text{vac}\rangle \tag{12.3}$$

$$= |\text{vac}\rangle - \frac{ig\alpha_3}{\hbar}\,|\text{Fock} : s=1, s=2\rangle\,, \tag{12.4}$$

where

$$|\text{Fock} : s=1, s=2\rangle \equiv \hat{a}_1^\dagger\hat{a}_2^\dagger\,|\text{vac}\rangle \tag{12.5}$$

is a **two-photon Fock state** that we discussed in Sec. 5.6, with one $\tilde{\boldsymbol{e}}_1$-polarized photon, denoted by $s=1$ in the notation, and one $\tilde{\boldsymbol{e}}_2$-polarized photon, denoted by $s=2$ (we omit the mention of the wavevectors for brevity). We see that the process creates two photons at half the frequency of the pump, hence the name spontaneous parametric down conversion (SPDC).

In the setup depicted by Fig. 12.1, there is another pump beam propagating in the $-\tilde{\boldsymbol{x}}$ direction. Let $\alpha_3 e^{i\theta}$ be its amplitude, $\hat{b}_1$ be the annihilation operator for another signal mode with polarization vector $\tilde{\boldsymbol{y}}$, and $\hat{b}_2$ be another idler mode with polarization vector $\tilde{\boldsymbol{z}}$. These three modes have the same properties as the three modes discussed earlier, except that they propagate in the opposite direction. The total Hamiltonian becomes

$$\hat{\eta}_{\text{easy}}(t) = g\alpha_3\left(\hat{a}_1^\dagger\hat{a}_2^\dagger + e^{i\theta}\hat{b}_1^\dagger\hat{b}_2^\dagger\right) + \text{H.c.}. \tag{12.6}$$

and the quantum state becomes

$$|\psi_I(t)\rangle \approx |\text{vac}\rangle - \frac{ig\alpha_3}{\hbar}\left(\hat{a}_1^\dagger\hat{a}_2^\dagger + e^{i\theta}\hat{b}_1^\dagger\hat{b}_2^\dagger\right)|\text{vac}\rangle\,. \tag{12.7}$$

Let's focus on the two-photon component:

$$\left|\psi_I^{(2)}(t)\right\rangle \propto \left(\hat{a}_1^\dagger\hat{a}_2^\dagger + e^{i\theta}\hat{b}_1^\dagger\hat{b}_2^\dagger\right)|\text{vac}\rangle = |\text{Fock} : s_a=1, s_a=2\rangle + e^{i\theta}\,|\text{Fock} : s_b=1, s_b=2\rangle\,. \tag{12.8}$$

This equation says that the two-photon state is a superposition of two possibilities:

(1) Two photons, one $\tilde{\boldsymbol{e}}_1$-polarized (denoted by $s_a = 1$) and one $\tilde{\boldsymbol{e}}_2$-polarized (denoted by $s_a = 2$), are propagating in the $+\tilde{\boldsymbol{x}}$ direction.
(2) Two photons, one $\tilde{\boldsymbol{e}}_1$-polarized (denoted by $s_b = 1$) and one $\tilde{\boldsymbol{e}}_2$-polarized (denoted by $s_b = 2$), are propagating in the $-\tilde{\boldsymbol{x}}$ direction.

The two counter-propagating beams then meet at a **polarizing beam splitter (PBS)**. Let's say the optical beam propagating in the $+\tilde{\boldsymbol{x}}$ direction is directed to the first input of the PBS, and the other beam is direct to the second input of the PBS. A PBS fully transmits one polarization, say, $\tilde{\boldsymbol{e}}_1$, and fully reflects the other polarization $\tilde{\boldsymbol{e}}_2$, as depicted in Fig. 12.2. Consider the following two cases:

(1) If two photons come into the first input:
  (a) The $\tilde{\boldsymbol{e}}_1$ photon is transmitted into the first output.
  (b) The $\tilde{\boldsymbol{e}}_2$ photon is reflected into the second output.
(2) If two photons come into the second input:
  (a) The $\tilde{\boldsymbol{e}}_1$ photon is transmitted into the second output.

(b) The $\tilde{e}_2$ photon is reflected into the first output.

In either case, there is always one photon in the first output and one photon in the second output. The polarization of each photon is unknown because we don't know whether the photon comes from the first input or the second input, but we know that, if the polarization of the first output is $\tilde{e}_1$, then the polarization of the second output must be $\tilde{e}_2$, and vice versa, because the photons, regardless of their origin, are created in a pair with orthogonal polarizations.

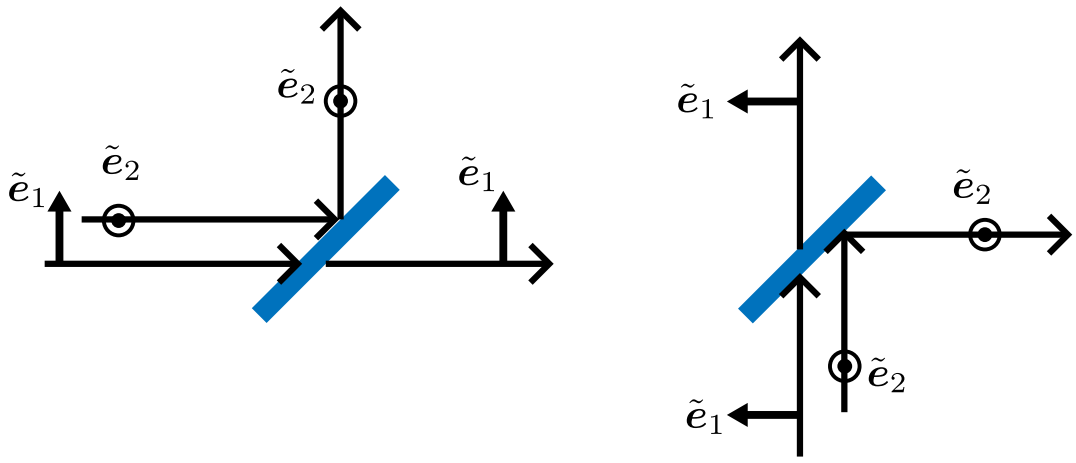

FIGURE 12.2. A polarizing beam splitter (PBS) fully transmits one polarization and fully reflects the other polarization.

We say that the polarizations of the two photons are **entangled**.

To model the physics mathematically, define the following:

(1) For the first output, let $\hat{c}_1$ and $\hat{c}_2$ be the operators for two polarization modes $\tilde{e}_1$ and $\tilde{e}_2$, respectively.
(2) For the second output, let $\hat{d}_1$ and $\hat{d}_2$ be the operators for two polarization modes $\tilde{e}_1$ and $\tilde{e}_2$, respectively.

Let $\hat{U}$ be the unitary operator for the PBS, which obeys passive linear optics. The input-output relation for the PBS in the Heisenberg picture can be taken as

$$\hat{c}_1(T) = \hat{U}^\dagger \hat{c}_1 \hat{U} = \hat{a}_1, \quad \hat{c}_2(T) = \hat{U}^\dagger \hat{c}_2 \hat{U} = \hat{b}_2, \quad \hat{d}_1(T) = \hat{U}^\dagger \hat{d}_1 \hat{U} = \hat{b}_1, \quad \hat{d}_2(T) = \hat{U}^\dagger \hat{d}_2 \hat{U} = \hat{a}_2. \tag{12.9}$$

In the Schrödinger picture, the two-photon component of the state hence becomes

$$\hat{U} \left|\psi_I^{(2)}\right\rangle \propto \hat{U}\left(\hat{a}_1^\dagger \hat{a}_2^\dagger + e^{i\theta}\hat{b}_1^\dagger \hat{b}_2^\dagger\right)|\text{vac}\rangle \tag{12.10}$$

$$= \left(\hat{U}\hat{a}_1^\dagger \hat{U}^\dagger \hat{U}\hat{a}_2^\dagger \hat{U}^\dagger + e^{i\theta}\hat{U}\hat{b}_1^\dagger \hat{U}^\dagger \hat{U}\hat{b}_2^\dagger \hat{U}^\dagger\right)\hat{U}|\text{vac}\rangle \tag{12.11}$$

$$= \left(\hat{c}_1^\dagger \hat{d}_2^\dagger + e^{i\theta}\hat{d}_1^\dagger \hat{c}_2^\dagger\right)|\text{vac}\rangle \quad \text{(using Eqs. (12.9) and } \hat{U}|\text{vac}\rangle = |\text{vac}\rangle) \tag{12.12}$$

$$\equiv |\text{Fock} : s_c = 1, s_d = 2\rangle + e^{i\theta}|\text{Fock} : s_c = 2, s_d = 1\rangle\,. \tag{12.13}$$

As advertised, this result shows that, given that there are two photons, there is always one photon in the $\hat{c}_{1,2}$ modes in the first output and one photon in the $\hat{d}_{1,2}$ modes in the second output. Moreover, their polarizations are entangled: If the first photon has polarization vector $\tilde{e}_1$ (denoted by $s_c = 1$), then the second photon has polarization vector $\tilde{e}_2$ (denoted by $s_d = 2$), and vice versa. The relative phase θ between the two possibilities can be controlled by optical components.

There are a variety of other methods and configurations to produce entangled photons, although most of them are based on SPDC in a $\chi^{(2)}$ crystal.

12.2. Bell's theorem and the CHSH game

A lot of people, including Einstein, are not happy with quantum mechanics and they suggest that there may be a deeper classical "hidden-variable" theory underlying quantum mechanics. Inspired by Einstein, Bell and others proposed experiments that can test those classical theories. They showed that, according to those classical theories, the experimental result must obey certain inequalities, while quantum mechanics can violate them. An experiment violating any of those inequalities can rule out a large class of classical hidden-variable theories in one go. Those inequalities are now commonly called Bell's theorem. See, for example, https://www.nobelprize.org/prizes/physics/2022/summary/ and Refs. [25, 26] for an introduction.

We will focus on one popular version of the inequalities called the CHSH inequality (named after its inventors Clauser, Horne, Shimony, and Holt) and treat the experiment as a game called the CHSH game. A nice video about the game can be found at https://www.youtube.com/watch?v=v7jctqKsUMA. Our description of the game below is slightly different from the video in order to make our description closer to the academic literature, although the essential idea is the same.

12.2.1. Rules of the CHSH game.

(1) The game involves two cooperating players, commonly called **Alice** and **Bob**, and a **referee**.
(2) After the game starts, Alice and Bob are separated and forbidden to communicate with each other. The referee can communicate with both.
(3) In each round of the game, the referee sends one random instruction u to Alice and another random instruction v to Bob. There are only two possible instructions "1" or "2" for each player, so in total there are 4 possible sets of instructions $(u, v) = (1, 1), (1, 2), (2, 1),$ or $(2, 2)$ sent to Alice and Bob, as shown in Table 1.
(4) After receiving the instruction, Alice should send an answer $A = +1$ or -1 to the referee.
(5) Similarly, Bob should also send an answer $B = +1$ or -1 to the referee.
(6) The reward is computed as follows:
   (a) If Alice and Bob receive the instructions $(1, 1)$, $(2, 1)$, or $(2, 2)$, they win a dollar if their answers are the same ($A = B$), or lose a dollar if their answers are different ($A \neq B$). The reward given such instructions is hence AB.
   (b) However, if they receive the instructions $(1, 2)$, they win a dollar if their answers are different ($A \neq B$), or lose a dollar if their answers are the same ($A = B$). The reward given such instructions is hence $-AB$.

   Table 1 summarizes the rules of the game.
(7) Many rounds of the game are played, and the instructions are random each time, i.e., the four sets of instructions $(1, 1), (1, 2), (2, 1), (2, 2)$ have equal probability $1/4$.

Instruction to Alice (u)	Instruction to Bob (v)	Win condition	Reward	Expected Reward
1	1	$A = B$	AB	$C_{11} \equiv \mathbb{E}(AB\|1, 1)$
1	2	$A \neq B$	$-AB$	$-C_{12} \equiv -\mathbb{E}(AB\|1, 2)$
2	1	$A = B$	AB	$C_{21} \equiv \mathbb{E}(AB\|2, 1)$
2	2	$A = B$	AB	$C_{22} \equiv \mathbb{E}(AB\|1, 2)$

TABLE 1. CHSH game rules.

We allow Alice and Bob to communicate **before** the game starts. We also allow Alice and Bob to adopt any deterministic or randomized strategy, i.e., A and B may be **random variables**, so that the *expected* reward given each set of instructions is listed in the last column of Table 1. The overall expected reward is hence

$$\boxed{\text{expected reward per round} = \frac{1}{4}\mathcal{S},} \tag{12.14}$$

where

$$\boxed{\mathcal{S} \equiv C_{11} - C_{12} + C_{21} + C_{22}} \tag{12.15}$$

is called **the CHSH number** and

$$\boxed{C_{uv} \equiv \mathbb{E}(AB|u,v)} \tag{12.16}$$

is the **correlation** of the players' answers given instructions (u, v). In other words, the players' answers should be as correlated as possible to maximize C_{11}, C_{21}, and C_{22}, except the $(1, 2)$ case, when they should be as anti-correlated as possible to minimize C_{12}.

By playing many rounds, the average reward should converge to the expected reward.

12.2.2. Classical: hidden-variable model. We first pretend that we don't know quantum mechanics and assume that Alice and Bob follow the laws of classical probability theory. We use one random variable λ, called the **hidden variable**, to denote any pre-shared information between them and also any random-number generator, e.g., dices, they use in determining their answers. We do not otherwise impose any restriction on λ; we allow its sample space to be arbitrary (e.g., λ can be a number or a vector of any dimension) and its probability distribution can also be arbitrary.

We also allow Alice and Bob to adopt any strategy, with the important restriction that they cannot know the instruction to the other player. Let $A_u(\lambda)$ be Alice's answer given instruction $u = 1$ or 2, and likewise $B_v(\lambda)$ be Bob's answer given instruction $v = 1$ or 2. Then we allow $A_u(\lambda)$ and $B_v(\lambda)$ to be arbitrary functions of the hidden variable λ. The correlation in Eq. (12.16) becomes

$$\boxed{C_{uv} = \mathbb{E}\left[A_u(\lambda)B_v(\lambda)\right].} \tag{12.17}$$

As proved in Sec. 12.2.3, the assumption of Eq. (12.17) under the hidden-variable model leads to an inequality for the CHSH number given by

$$\boxed{|\mathcal{S}| \le 2.} \tag{12.18}$$

This inequality is called the **CHSH inequality** after its inventors (https://en.wikipedia.org/wiki/CHSH_inequality). In the context of the game, the inequality means that the expected reward per round $\mathcal{S}/4$ cannot exceed $2/4 = 0.5$. (It also means that the expected reward cannot go below $-2/4 = -0.5$.)

We have assumed very little about the hidden-variable model for the proof of the CHSH inequality—the model allows Alice and Bob to pre-share any classical data and use any strategy. The hidden-variable model is sometimes called **local realism**; it encapsulates many physicists' belief about the fundamental properties of all physical objects, including our Alice and Bob. I won't go into the philosophical details and simply refer you to Refs. [25, 26] for more information.

12.2.3. Side note: Proof of CHSH inequality (12.18). I follow Wikipedia https://en.wikipedia.org/wiki/CHSH_inequality#Bell's_1971_derivation. First consider

$$\begin{aligned} C_{11} - C_{12} &= \mathbb{E}\left(A_1B_1 - A_1B_2\right) = \mathbb{E}\left(A_1B_1 - A_1B_2 \pm A_1B_1A_2B_2 \mp A_1B_1A_2B_2\right) && (12.19)\\ &= \mathbb{E}\left[A_1B_1(1 \pm A_2B_2)\right] - \mathbb{E}\left[A_1B_2(1 \pm A_2B_1)\right]. && (12.20) \end{aligned}$$

Take absolute values of both sides, and use triangle inequality $|x + y| \le |x| + |y|$ and Jensen's inequality $\mathbb{E}(|X|) \le |\mathbb{E}(X)|$ (https://en.wikipedia.org/wiki/Jensen%27s_inequality):

$$\begin{aligned} |C_{11} - C_{12}| &\le |\mathbb{E}\left[A_1B_1(1 \pm A_2B_2)\right]| + |\mathbb{E}\left[A_1B_2(1 \pm A_2B_1)\right]| && \text{(triangle ineq.)} && (12.21)\\ &\le \mathbb{E}\left[|A_1B_1(1 \pm A_2B_2)|\right] + \mathbb{E}\left[|A_1B_2(1 \pm A_2B_1)|\right] && \text{(Jensen)} && (12.22)\\ &= \mathbb{E}\left(|A_1B_1||1 \pm A_2B_2|\right) + \mathbb{E}\left(|A_1B_2||1 \pm A_2B_1|\right) && && (12.23)\\ &\le \mathbb{E}\left(|1 \pm A_2B_2|\right) + \mathbb{E}\left(|1 \pm A_2B_1|\right) && (|A_jB_l| \le 1) && (12.24)\\ &= \mathbb{E}\left(1 \pm A_2B_2\right) + \mathbb{E}\left(1 \pm A_2B_1\right) && (1 \pm A_jB_l \ge 0) && (12.25)\\ &= 2 \pm C_{22} \pm C_{21} = 2 \pm (C_{21} + C_{22}). && && (12.26) \end{aligned}$$

It follows that

$$|C_{11} - C_{12}| \le 2 - |C_{21} + C_{22}|, \tag{12.27}$$

$$|C_{11} - C_{12}| + |C_{21} + C_{22}| \le 2, \tag{12.28}$$

$$|C_{11} - C_{12} + C_{21} + C_{22}| \le |C_{11} - C_{12}| + |C_{21} + C_{22}| \le 2. \qquad \text{(triangle ineq.)} \tag{12.29}$$

12.2.4. Quantum: better strategy using entanglement. The hidden-variable model sounds general and reasonable, but it turns out that Alice and Bob can do better in the game and violate the CHSH inequality if they share entanglement.

(1) For each round, Alice has a photon and Bob has a photon. The photons are entangled in their polarizations.
(2) After receiving an instruction, Alice measures the polarization of her photon with respect to the two possible polarization vectors

$$\tilde{\boldsymbol{e}}_+(a) = (\cos a)\tilde{\boldsymbol{y}} + (\sin a)\tilde{\boldsymbol{z}}, \qquad \tilde{\boldsymbol{e}}_-(a) = (-\sin a)\tilde{\boldsymbol{y}} + (\cos a)\tilde{\boldsymbol{z}}, \tag{12.30}$$

where **Alice's measurement setting** $a = a_u$ depends on the instruction u she receives.
(3) Her answer A depends on the measurement outcome:
  (a) if the photon is found to have polarization $\tilde{\boldsymbol{e}}_+(a)$, $A = +1$,
  (b) if the photon is found to have polarization $\tilde{\boldsymbol{e}}_-(a)$, $A = -1$.
(4) Similarly, Bob measures the polarization with respect to the polarization vectors

$$\tilde{\boldsymbol{e}}_+(b) = (\cos b)\tilde{\boldsymbol{y}} + (\sin b)\tilde{\boldsymbol{z}}, \qquad \tilde{\boldsymbol{e}}_-(b) = (-\sin b)\tilde{\boldsymbol{y}} + (\cos b)\tilde{\boldsymbol{z}}, \tag{12.31}$$

where **Bob's measurement setting** $b = b_v$ depends on the instruction v he receives.
(5) His answer B depends on the measurement outcome in the same way as Alice's:
  (a) if the photon is found to have polarization $\tilde{\boldsymbol{e}}_+(b)$, $B = +1$,
  (b) if the photon is found to have polarization $\tilde{\boldsymbol{e}}_-(b)$, $B = -1$.
(6) Many rounds of the game are played, and the average reward should converge to the expected reward.

With entangled photons, it turns out to be possible for $\mathcal{S}$ to violate the CHSH inequality $|\mathcal{S}| \le 2$ given by Eq. (12.18) and for the players to obtain a higher ($\mathcal{S} > 2$, $\mathcal{S}/4 > 0.5$) or lower ($\mathcal{S} < -2$, $\mathcal{S}/4 < -0.5$) expected reward for the game.

A and B are still random variables in quantum mechanics, although their joint probability distribution, conditioned on the settings (a, b), should be computed from

$$P(A, B|a, b) = |\langle \text{Fock} : A, a; B, b|\psi\rangle|^2 = \left|\langle \text{vac}|\, \hat{c}_A(a)\hat{d}_B(b)\, |\psi\rangle\right|^2, \tag{12.32}$$

where

(1) $|\psi\rangle$ is the quantum state of the entangled photons,
(2) $|\text{Fock} : A, a; B, b\rangle = \hat{c}_A^\dagger(a)\hat{d}_B^\dagger(b)\,|\text{vac}\rangle$ is a two-photon state where Alice's photon has polarization $\tilde{\boldsymbol{e}}_A(a)$ and Bob's photon has polarization $\tilde{\boldsymbol{e}}_B(b)$,
(3) the new polarization-mode operators, according to Sec. 3.5.1, should be defined as

$$\hat{c}_+(a) \equiv (\cos a)\hat{c}_1 + (\sin a)\hat{c}_2, \qquad \hat{d}_+(b) \equiv (\cos b)\hat{d}_1 + (\sin b)\hat{d}_2, \tag{12.33}$$

$$\hat{c}_-(a) \equiv -(\sin a)\hat{c}_1 + (\cos a)\hat{c}_2, \qquad \hat{d}_-(b) \equiv -(\sin b)\hat{d}_1 + (\cos b)\hat{d}_2. \tag{12.34}$$

The correlation in Eq. (12.16) becomes

$$C_{uv} \equiv \mathbb{E}\,(AB|u, v) = \sum_{A=\pm1, B=\pm1} ABP(A, B|a_u, b_v). \tag{12.35}$$

We can no longer assume Eq. (12.17) under the hidden-variable model, where A is a function of Alice's instruction u only and B is a function of Bob's instruction v only. Here we must take both instructions (u, v) into account when computing each correlation.

We now study a specific quantum scenario that can violate the CHSH inequality (12.18). Let the quantum state be

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger \hat{d}_2^\dagger - \hat{c}_2^\dagger \hat{d}_1^\dagger\right)|\text{vac}\rangle\,, \tag{12.36}$$

where I've assumed $e^{i\theta} = -1$, so that the state is the so-called singlet state (https://en.wikipedia.org/wiki/Singlet_state). (I also ignore the events when no photon comes in so that the post-selected quantum state is the two-photon state without the $|\text{vac}\rangle$ component.) The probabilities of detecting the two photons in certain pairs of polarizations become

$$P(1,1|a,b) = \left|\langle\text{vac}|\,\hat{c}_+\hat{d}_+\,|\psi\rangle\right|^2 = \left|\langle\text{vac}|\,\hat{c}_+\hat{d}_+\frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger \hat{d}_2^\dagger - \hat{c}_2^\dagger \hat{d}_1^\dagger\right)|\text{vac}\rangle\right|^2 \tag{12.37}$$

$$= \frac{1}{2}[(\cos a)(\sin b) - (\sin a)(\cos b)]^2 = \frac{1}{2}\sin^2(a-b), \tag{12.38}$$

$$P(1,-1|a,b) = \left|\langle\text{vac}|\,\hat{c}_+\hat{d}_-\,|\psi\rangle\right|^2 = \left|\langle\text{vac}|\,\hat{c}_+\hat{d}_-\frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger \hat{d}_2^\dagger - \hat{c}_2^\dagger \hat{d}_1^\dagger\right)|\text{vac}\rangle\right|^2 \tag{12.39}$$

$$= \frac{1}{2}[(\cos a)(\cos b) - (\sin a)(-\sin b)]^2 = \frac{1}{2}\cos^2(a-b), \tag{12.40}$$

$$P(-1,1|a,b) = \left|\langle\text{vac}|\,\hat{c}_-\hat{d}_+\,|\psi\rangle\right|^2 = \left|\langle\text{vac}|\,\hat{c}_-\hat{d}_+\frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger \hat{d}_2^\dagger - \hat{c}_2^\dagger \hat{d}_1^\dagger\right)|\text{vac}\rangle\right|^2 \tag{12.41}$$

$$= \frac{1}{2}[-(\sin a)(\sin b) - (\cos a)(\cos b)]^2 = \frac{1}{2}\cos^2(a-b), \tag{12.42}$$

$$P(-1,-1|a,b) = \left|\langle\text{vac}|\,\hat{c}_-\hat{d}_-\,|\psi\rangle\right|^2 = \left|\langle\text{vac}|\,\hat{c}_-\hat{d}_-\frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger \hat{d}_2^\dagger - \hat{c}_2^\dagger \hat{d}_1^\dagger\right)|\text{vac}\rangle\right|^2 \tag{12.43}$$

$$= \frac{1}{2}[(-\sin a)(\cos b) - (\cos a)(-\sin b)]^2 = \frac{1}{2}\sin^2(a-b). \tag{12.44}$$

The correlation $C(a,b)$ given settings (a,b) becomes

$$C(a,b) \equiv \sum_{A,B} ABP(A,B|a,b) \tag{12.45}$$

$$= P(1,1|a,b) - P(1,-1|a,b) - P(-1,1|a,b) + P(-1,-1|a,b) \tag{12.46}$$

$$= \sin^2(a-b) - \cos^2(a-b) = -\cos[2(a-b)]. \tag{12.47}$$

Notice the following special cases:

(1) When $a = b$, $P(1,1|a,a) = P(-1,-1|a,a) = 0$, $P(1,-1|a,a) = P(-1,1|a,a) = 1/2$, and $C(a,a) = -1$, indicating that the polarizations of the photon pair are always orthogonal to each other, regardless of a. This is a special property of the singlet state.
(2) When $a - b = \pi/4$, Bob's polarization vectors are rotated by 45° with respect to Alice's, and $C(a,b) = 0$.
(3) When $a - b = \pi/2$, Bob's polarization vectors are rotated by 90° with respect to Alice's, and $C(a,b) = 1$.

To compute the CHSH number given by Eq. (12.15), we combine Eqs. (12.35) and (12.45) to write $C_{uv} = C(a_u, b_v)$ and choose the settings

$$a_1 = 0, \qquad a_2 = \frac{\pi}{4}, \qquad b_1 = \frac{\pi}{8}, \qquad b_2 = \frac{3\pi}{8}. \tag{12.48}$$

Then

$$C_{11} = C(a_1,b_1) = -\frac{1}{\sqrt{2}}, \qquad C_{12} = C(a_1,b_2) = \frac{1}{\sqrt{2}}, \tag{12.49}$$

$$C_{21} = C(a_2,b_1) = -\frac{1}{\sqrt{2}}, \qquad C_{22} = C(a_2,b_2) = -\frac{1}{\sqrt{2}}, \tag{12.50}$$

leading to

$$\boxed{\mathcal{S} = -2\sqrt{2}.} \tag{12.51}$$

Hence $|\mathcal{S}| > 2$, which violates the CHSH inequality (12.18). In the context of the game, $\mathcal{S} < -2$ means that the expected reward goes below the minimum allowed by the hidden-variable model.

To demonstrate the violation of the CHSH inequality experimentally, many entangled photon pairs are measured (many rounds of the game are played) so that the reward, based on the measurement outcomes and averaged over the many rounds, should violate the CHSH inequality for the expected reward $|\mathcal{S}|/4 \leq 0.5$ significantly. There are many other entangled states and settings that allow one to violate the CHSH inequality, but the key ingredient of the experiment is the entangled photons.

People often borrow Einstein's phrase "*spooky action at a distance*" to describe the violation of local realism. For a lot of people, a conclusive experiment that violates local realism is a big deal [25, 26], so much so that they managed to convince the Nobel committee to award the key experimentalists Clauser, Aspect, and Zeilinger a Nobel Prize in Physics (https://www.nobelprize.org/prizes/physics/2022/summary/).

Exercise 12.1. Verify Eqs. (12.37)–(12.44).

Exercise 12.2. Show that C_{uv} can also be expressed as

$$C_{uv} = \langle\psi| \hat{A}_u \otimes \hat{B}_v |\psi\rangle , \tag{12.52}$$

where $\hat{A}_u$ and $\hat{B}_v$ are observables you should find.

(The expression now looks closer to Eq. (12.17) under the hidden-variable model, although still not the same, because the probability distribution of $(\hat{A}_u, \hat{B}_v)$ still depends on (u, v) afterall.)

Exercise 12.3. Using quantum theory, compute the marginal probability distribution of Alice's outcome:

$$\sum_B P(A, B|a, b) \tag{12.53}$$

and show that it does not depend on b. Do the same for Bob's outcome.

(This exercise shows that Bob's setting b cannot influence the statistics of A and Alice cannot learn anything about b if she's alone; same for Bob, so the entangled photons do not allow them to communicate via their settings. The violation of Bell's theorem can be revealed only after the referee has combined their results or Alice and Bob have come together to combine their results.)

Exercise 12.4. Let

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger \hat{d}_2^\dagger + e^{i\theta}\hat{c}_2^\dagger \hat{d}_1^\dagger\right)|\text{vac}\rangle , \tag{12.54}$$

$$\hat{c}_+ = (\cos a)\hat{c}_1 + (e^{i\phi}\sin a)\hat{c}_2, \tag{12.55}$$

$$\hat{c}_- = (-e^{-i\phi}\sin a)\hat{c}_1 + (\cos a)\hat{c}_2, \tag{12.56}$$

$$\hat{d}_+ = (\cos b)\hat{d}_1 + (e^{i\phi}\sin b)\hat{d}_2, \tag{12.57}$$

$$\hat{d}_- = (-e^{-i\phi}\sin b)\hat{d}_1 + (\cos b)\hat{d}_2. \tag{12.58}$$

Suppose that experimentalists tell you θ and ϕ are some real constants that they cannot change. Compute $C(a, b)$ and give them a set of settings $(a_1, b_1), (a_1, b_2), (a_2, b_1), (a_2, b_2)$ such that $|\mathcal{S}| = 2\sqrt{2}$.

Exercise 12.5. To measure a photon in a certain polarization basis, one way is to use a quarter-wave plate (QWP), an electro-optic modulator (EOM), and a PBS shown in Fig. 12.3.

(1) The QWP applies a phase shift ϕ_0 to the $\tilde{\mathbf{e}}_1$-polarization mode and a phase shift $\phi_0 + \pi/2$ to the $\tilde{\mathbf{e}}_2$-polarization mode.

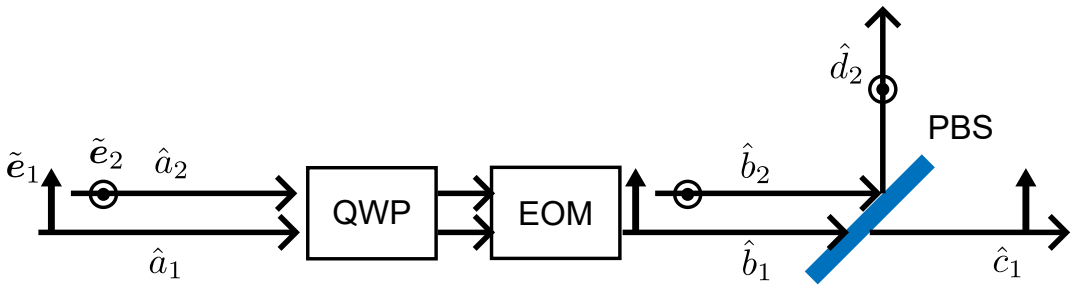

FIGURE 12.3.

(2) The EOM applies a phase shift ϕ_1 to the $\tilde{\boldsymbol{e}}_+$-polarization mode and a different phase shift ϕ_2 to the $\tilde{\boldsymbol{e}}_-$-polarization mode, where

$$\tilde{\boldsymbol{e}}_+ \equiv \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{e}}_1 + \tilde{\boldsymbol{e}}_2), \qquad \tilde{\boldsymbol{e}}_- \equiv \frac{1}{\sqrt{2}}(\tilde{\boldsymbol{e}}_1 - \tilde{\boldsymbol{e}}_2). \tag{12.59}$$

Let $\hat{a}_{1,2}$ be the operator for the $\tilde{\boldsymbol{e}}_{1,2}$-polarized mode at the input and $\hat{b}_{1,2}(T)$ be the operator for the $\tilde{\boldsymbol{e}}_{1,2}$-polarized mode at the output.

(1) Find the input-output relation between $\begin{pmatrix}\hat{b}_1(T)\\ \hat{b}_2(T)\end{pmatrix} \equiv \begin{pmatrix}\hat{U}^\dagger \hat{b}_1 \hat{U}\\ \hat{U}^\dagger \hat{b}_2 \hat{U}\end{pmatrix}$ and $\begin{pmatrix}\hat{a}_1\\ \hat{a}_2\end{pmatrix}$, where $\hat{U}$ is the unitary operator that models the QWP + EOM setup.

(2) Let a one-photon state be

$$|\psi\rangle = \left(\psi_1 \hat{a}_1^\dagger + \psi_2 \hat{a}_2^\dagger\right)|\text{vac}\rangle\,. \tag{12.60}$$

Find the probability $P(+) = \left|\langle \text{Fock} : 1|\, \hat{U}\, |\psi\rangle\right|^2$ of detecting the photon in the $\hat{b}_1$ mode, where $|\text{Fock} : 1\rangle \equiv \hat{b}_1^\dagger |\text{vac}\rangle$, and the probability $P(+) = \left|\langle \text{Fock} : 2|\, \hat{U}\, |\psi\rangle\right|^2$ of detecting the photon in the $\hat{b}_2$ mode, where $|\text{Fock} : 2\rangle \equiv \hat{b}_2^\dagger |\text{vac}\rangle$.

(3) We would like to implement a measurement with respect to the basis $\{|\text{Fock} : +\rangle\,, |\text{Fock}, -\rangle\}$, where

$$|\text{Fock} : +\rangle = \hat{a}_+^\dagger |\text{vac}\rangle\,, \qquad |\text{Fock} : -\rangle = \hat{a}_-^\dagger |\text{vac}\rangle\,, \tag{12.61}$$

$$\hat{a}_+ = (\cos a)\hat{a}_1 + (\sin a)\hat{a}_2, \qquad \hat{a}_- = -(\sin a)\hat{a}_1 + (\cos a)\hat{a}_2, \tag{12.62}$$

and a is a given real number, so that the probabilities are given by $P(+) = |\langle +|\psi\rangle|^2$ and $P(-) = |\langle -|\psi\rangle|^2$, respectively. Find a set of ϕ_0, ϕ_1, ϕ_2 that implement the measurement.

CHAPTER 13

Incoherent Imaging*

Our goal in this chapter is to model the quantum state of light in an imaging system with incoherent sources for astronomy and fluorescence microscopy. The general idea is sketched in Fig. 13.1, which generalizes the two-input-two-output relations we studied earlier in Chapter 6. Multiple optical pulse modes on an input plane at $z = z_1$ propagate through passive linear optics. They are transformed to optical pulse modes on an output plane at $z = z_2 > z_1$ some time later. Let $\{\hat{f}_l\}$ be the annihilation operators for the input pulse modes and $\{\hat{g}_l\}$ be the annihilation operators for the output pulse modes. If the optics is lossless, the input-output relations in the Heisenberg picture are given by

$$\hat{g}_l = \sum_m V_{lm} \hat{f}_m, \tag{13.1}$$

where V is a unitary matrix, as we learned in Chapter 6. If there is loss, we assume that some modes are inaccessible and trace them out, following Chapter 7.

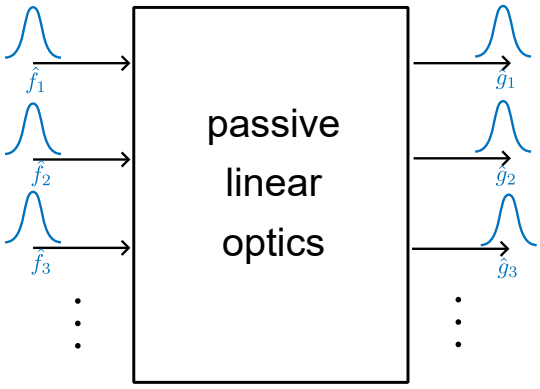

FIGURE 13.1. An imaging system as a multi-input-multi-output system. Multiple spatiotemporal modes with annihilation operators $\{\hat{f}_l\}$ are prepared at an input plane $z = z_1$, which are transformed to multiple spatiotemporal modes with operators $\{\hat{g}_l\}$ in the Heisenberg picture.

13.1. Spatiotemporal modes

13.1.1. Change of variables. The simple pulse modes we studied earlier assume $(k_x, k_y) = (0, 0)$ and $s = 1$. The electric fields of the modes look like pulses moving along z but are otherwise uniform along (x, y). To model imaging, we need to consider modes with more complicated spatial behavior. To define the modes in a way relatable to classical optics, we perform a change of variables from (k_x, k_y, k_z) to (k_x, k_y, ω), similar to what we did in Sec. 6.4.

Assume that the $(\boldsymbol{k}, s)$-space amplitude of a mode is nonzero only for $k_z > 0$, so that the mode propagates in the positive z direction. k_z can then be expressed as a function of (k_x, k_y, ω):

$$\boxed{k_z(k_x, k_y, \omega) = \sqrt{\left(\frac{\omega}{c}\right)^2 - k_x^2 - k_y^2}.} \tag{13.2}$$

Recall the annihilation operator $\hat{a}(\boldsymbol{k}, s)$ in the continuum case in Sec. 3.4. It satisfies the standard commutation relation $\left[\hat{a}(\boldsymbol{k}, s), \hat{a}^\dagger(\boldsymbol{k}', s')\right] = \delta^3(\boldsymbol{k} - \boldsymbol{k}')\delta_{ss'}$. In terms of the new variables, we define a new annihilation operator as

$$\hat{b}(k_x, k_y, \omega, s) \equiv \sqrt{\frac{\partial k_z(k_x, k_y, \omega)}{\partial \omega}} \hat{a}(k_x, k_y, k_z(k_x, k_y, \omega), s), \tag{13.3}$$

so that it satisfies a similar commutation relation

$$\boxed{\left[\hat{b}(\boldsymbol{\kappa}, s), \hat{b}^\dagger(\boldsymbol{\kappa}', s')\right] = \delta^3(\boldsymbol{\kappa} - \boldsymbol{\kappa}')\delta_{ss'},} \tag{13.4}$$

where we have defined the shorthands

$$\boldsymbol{\kappa} \equiv (k_x, k_y, \omega), \qquad \delta^3(\boldsymbol{\kappa} - \boldsymbol{\kappa}') \equiv \delta(k_x - k_x')\delta(k_y - k_y')\delta(\omega - \omega'). \tag{13.5}$$

We can now define an optical mode with mode label l by the annihilation operator

$$\boxed{\hat{f}_l = \sum_s \iiint W_l^*(\boldsymbol{k}, s)\hat{a}(\boldsymbol{k}, s)d^3\boldsymbol{k} = \sum_s \iiint \mathcal{W}_l^*(\boldsymbol{\kappa}, s)\hat{b}(\boldsymbol{\kappa}, s)d^3\boldsymbol{\kappa},} \tag{13.6}$$

where

$$d^3\boldsymbol{\kappa} \equiv dk_x dk_y d\omega, \qquad \iiint (\dots) d^3\boldsymbol{\kappa} \equiv \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty (\dots) dk_x dk_y d\omega, \tag{13.7}$$

$W_l(\boldsymbol{k}, s)$ is the continuum limit ($L \to \infty$) of $W_{jl}\Delta k^{-3/2}$ with $\Delta k \equiv 2\pi/L$, and

$$\boxed{\mathcal{W}_l(\boldsymbol{\kappa}, s) \equiv \sqrt{\frac{\partial k_z}{\partial \omega}} W_l(\boldsymbol{k}, s)} \tag{13.8}$$

is the $(\boldsymbol{\kappa}, s)$-space amplitude of the mode, obtained by substituting k_z with the function $k_z(k_x, k_y, \omega)$ on the right-hand side.

For a set of modes, their operators should satisfy the usual commutation relation

$$\left[\hat{f}_l, \hat{f}_m^\dagger\right] = \delta_{lm}, \tag{13.9}$$

so the amplitudes should satisfy the orthonormal condition

$$\boxed{\sum_s \iiint W_l^*(\boldsymbol{k}, s)W_m(\boldsymbol{k}, s)d^3\boldsymbol{k} = \sum_s \iiint \mathcal{W}_l^*(\boldsymbol{\kappa}, s)\mathcal{W}_m(\boldsymbol{\kappa}, s)d^3\boldsymbol{\kappa} = \delta_{lm}.} \tag{13.10}$$

We can study the physical meaning of the $(\boldsymbol{\kappa}, s)$-space amplitude $\mathcal{W}_l$ by considering the Heisenberg-picture electric field $\hat{\boldsymbol{E}}(\boldsymbol{r}, t)$ of the mode. It will be convenient to write the electric field as a sum of two parts:

$$\hat{\boldsymbol{E}}(\boldsymbol{r}, t) = \hat{\boldsymbol{E}}^{(+)}(\boldsymbol{r}, t) + \hat{\boldsymbol{E}}^{(-)}(\boldsymbol{r}, t), \tag{13.11}$$

where $\hat{\boldsymbol{E}}^{(+)}$ is called the positive-frequency part, given by

$$\hat{\boldsymbol{E}}^{(+)}(\boldsymbol{r}, t) \equiv \frac{1}{L^{3/2}} \sum_j \left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2} \hat{a}_j \tilde{\boldsymbol{e}}_{\boldsymbol{k},s} e^{i\boldsymbol{k}\cdot\boldsymbol{r} - i\omega_j t}, \tag{13.12}$$

and $\hat{\boldsymbol{E}}^{(-)}(\boldsymbol{r}, t) = [\hat{\boldsymbol{E}}^{(+)}(\boldsymbol{r}, t)]^\dagger$, the negative-frequency part, is simply the Hermitian conjugate of the former. With $\hat{a}_j = \sum_l W_{jl}\hat{f}_l$, we can write $\hat{\boldsymbol{E}}^{(+)}$ as

$$\hat{\boldsymbol{E}}^{(+)}(\boldsymbol{r}, t) = \sum_l \hat{f}_l \boldsymbol{v}_l(\boldsymbol{r}, t), \tag{13.13}$$

where the mode function $\boldsymbol{v}_l(\boldsymbol{r},t)$ is given by

$$\boldsymbol{v}_l(\boldsymbol{r},t) = \frac{1}{L^{3/2}}\sum_j \left(\frac{\hbar\omega_j}{2\epsilon_0}\right)^{1/2} W_{jl}\tilde{\boldsymbol{e}}_{\boldsymbol{k},s} e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\omega_j t} \tag{13.14}$$

$$\to \frac{1}{(2\pi)^{3/2}}\sum_s \iiint \left[\frac{\hbar\omega(\boldsymbol{k})}{2\epsilon_0}\right]^{1/2} W_l(\boldsymbol{k},s)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s} e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\omega(\boldsymbol{k})t} d^3\boldsymbol{k} \qquad (L\to\infty) \tag{13.15}$$

$$= \frac{1}{(2\pi)^{3/2}}\sum_s \iiint \left(\frac{\hbar\omega}{2\epsilon_0}\frac{\partial k_z}{\partial\omega}\right)^{1/2} \mathcal{W}_l(\boldsymbol{\kappa},s)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s} e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\omega t} d^3\boldsymbol{\kappa}. \tag{13.16}$$

Thus, (k_x,k_y,ω) are frequencies of a plane wave that determine the oscillations of the electric field along (x,y,t), and the integral represents a superposition of the plane waves over a range of (k_x,k_y,ω). It is customary in optics to specify a **spatiotemporal mode** by its mode function $\boldsymbol{v}_l(x,y,z=0,t)$ as a function of (x,y,t) at a fixed z. Given such a mode function, we can retrieve the $(\boldsymbol{\kappa},s)$-space amplitude by Fourier transform:

$$\mathcal{V}_l(\boldsymbol{\kappa},s) \equiv \frac{1}{(2\pi)^{3/2}}\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\cdot\iiint \boldsymbol{v}_l(x,y,z=0,t)\exp(-ik_x x - ik_y y + i\omega t)dxdydt \tag{13.17}$$

$$= \left(\frac{\hbar\omega}{2\epsilon_0}\frac{\partial k_z}{\partial\omega}\right)^{1/2}\mathcal{W}_l(\boldsymbol{\kappa},s), \tag{13.18}$$

$$\mathcal{W}_l(\boldsymbol{\kappa},s) = \left(\frac{\hbar\omega}{2\epsilon_0}\frac{\partial k_z}{\partial\omega}\right)^{-1/2}\mathcal{V}_l(\boldsymbol{\kappa},s). \tag{13.19}$$

13.1.2. Narrowband approximations. To proceed further, it will be convenient to make a couple of simplifying approximations that are common in optics:

(1) **Quasimonochromatic**: $\mathcal{W}_l(\boldsymbol{\kappa},s)$ is highly concentrated near a carrier frequency $\omega=\Omega$, and the bandwidth of $\mathcal{W}_l$ along ω is much smaller than Ω.

(2) **Paraxial**: $\mathcal{W}_l(\boldsymbol{\kappa},s)$ is highly concentrated near $(k_x,k_y)=(0,0)$, so that the mode consists mostly of plane waves with wavevectors that have small angles with the $\tilde{\boldsymbol{z}}$ axis. In other words, we assume

$$\sqrt{k_x^2+k_y^2} \ll \frac{\Omega}{c}. \tag{13.20}$$

We call these the **narrowband** approximations. They mean that $\mathcal{W}_l(\boldsymbol{\kappa},s)$ is highly concentrated near

$$(k_x,k_y,\omega) = (0,0,\Omega) \tag{13.21}$$

and $W_l(\boldsymbol{k},s)$ in $\boldsymbol{k}$ space is highly concentrated near $(k_x,k_y,k_z)=(0,0,\Omega/c)$; see Fig. 13.2. We can then assume

$$\frac{\hbar\omega}{2\epsilon_0}\frac{\partial k_z}{\partial\omega} \approx \frac{\hbar\Omega}{2\epsilon_0 c}, \qquad \tilde{\boldsymbol{e}}_{\boldsymbol{k},1}\approx\tilde{\boldsymbol{e}}_{k\tilde{\boldsymbol{z}},1}, \qquad \tilde{\boldsymbol{e}}_{\boldsymbol{k},2}\approx\tilde{\boldsymbol{e}}_{k\tilde{\boldsymbol{z}},2}, \tag{13.22}$$

so that the cumbersome prefactor in Eq. (13.19) is a constant, we can treat $\mathcal{W}_l(\boldsymbol{\kappa},s)$ as the Fourier transform of the mode function $\boldsymbol{v}_l(\boldsymbol{r},t)$, and the polarization vectors do not depend on the wavevector and we can write $\tilde{\boldsymbol{e}}_{k\tilde{\boldsymbol{z}},s}=\tilde{\boldsymbol{e}}_s$ in the following. One possible choice is

$$\tilde{\boldsymbol{e}}_1 = \tilde{\boldsymbol{x}}, \qquad \tilde{\boldsymbol{e}}_2 = \tilde{\boldsymbol{y}}, \tag{13.23}$$

but any pair of orthonormal vectors perpendicular to $\tilde{\boldsymbol{z}}$ will do.

13.1.3. Mode amplitude in real space and time. It is often more intuitive to work in real space and time. Abbreviate the coordinates (x,y,t) as

$$\boldsymbol{\xi} \equiv (x,y,t) \tag{13.24}$$

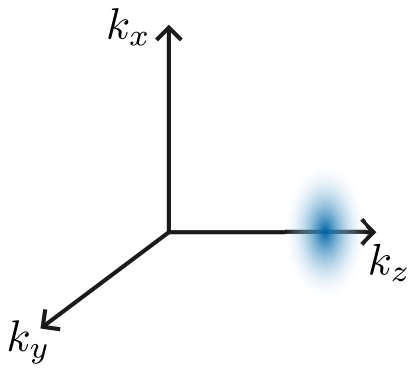

FIGURE 13.2. The narrowband approximations mean that the $(\boldsymbol{k}, s)$-space amplitude $W_l(\boldsymbol{k}, s)$ is highly concentrated near $(k_x, k_y, k_z) = (0, 0, \Omega/c)$ in $\boldsymbol{k}$ space.

and define the $(\boldsymbol{\xi}, s)$-space amplitude of the mode as the inverse Fourier transform

$$\boxed{w_l(\boldsymbol{\xi}, s) \equiv \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{W}_l(k_x, k_y, \Omega + \tilde{\omega}, s) \exp(ik_x x + ik_y y - i\tilde{\omega}t) dk_x dk_y d\tilde{\omega},} \tag{13.25}$$

where we have defined

$$\tilde{\omega} \equiv \omega - \Omega, \tag{13.26}$$

as the frequency relative to the carrier. We can take the integration limits with respect to $\tilde{\omega}$ to be $(-\infty, \infty)$ because $\mathcal{W}_l \approx 0$ outside a narrow band centered at the carrier Ω. This definition means that $w_l(\boldsymbol{\xi}, s)$ is the inverse Fourier transform of a function $W_l(k_x, k_y, \Omega + \tilde{\omega}, s)$ that is concentrated near $(k_x, k_y, \tilde{\omega}) = (0, 0, 0)$ with a small bandwidth, so w_l is **slowly varying** in (x, y, t) relative to the frequencies Ω/c in space and Ω in time.

Side note. *In optics, another name for $w_l(\boldsymbol{\xi}, s)$ is the envelope function of the mode, and the narrowband approximation is also called the slowly-varying-envelope approximation.*

By Fourier duality,

$$\mathcal{W}_l(k_x, k_y, \Omega + \tilde{\omega}, s) = \frac{1}{(2\pi)^{3/2}} \iiint w_l(\boldsymbol{\xi}, s) \exp(-ik_x x - ik_y y + i\tilde{\omega}t) d^3\boldsymbol{\xi}, \tag{13.27}$$

so the annihilation operator for the mode given by Eq. (13.6) can also be expressed as

$$\hat{f}_l = \sum_s \iiint w_l^*(\boldsymbol{\xi}, s) \hat{c}(\boldsymbol{\xi}, s) d^3\boldsymbol{\xi}, \tag{13.28}$$

where

$$\hat{c}(\boldsymbol{\xi}, s) \equiv \frac{1}{(2\pi)^{3/2}} \iiint \hat{b}(k_x, k_y, \Omega + \tilde{\omega}, s) e^{ik_x x + ik_y y - i\tilde{\omega}t} dk_x dk_y d\tilde{\omega}, \tag{13.29}$$

$$\left[\hat{c}(\boldsymbol{\xi}, s), \hat{c}^\dagger(\boldsymbol{\xi}', s')\right] = \delta^3(\boldsymbol{\xi} - \boldsymbol{\xi}') \delta_{ss'}. \tag{13.30}$$

By virtue of Parseval's theorem, the $(\boldsymbol{\xi}, s)$-space amplitudes for a set of modes are orthonormal in the sense of

$$\boxed{\sum_s \iiint w_l^*(\boldsymbol{\xi}, s) w_m(\boldsymbol{\xi}, s) d^3\boldsymbol{\xi} = \delta_{lm}.} \tag{13.31}$$

Using Eqs. (13.16) and (13.25) and making the narrowband approximations, the electric field of the mode can now be expressed as

$$\boxed{\boldsymbol{v}_l(x,y,z=0,t) \approx \left(\frac{\hbar\Omega}{2\epsilon_0 c}\right)^{1/2} \sum_s \tilde{\boldsymbol{e}}_s w_l(\boldsymbol{\xi},s) e^{-i\Omega t},} \tag{13.32}$$

so that the $w_l(\boldsymbol{\xi},s)$ amplitude is more directly related to the electric field in real space and time. Examples:

(1) A monochromatic point source at position $(x,y,z)=(u,v,0)$ would excite a mode with an amplitude $w_l(\boldsymbol{\xi},s)$ that is highly concentrated near $(x,y)=(u,v)$ at $z=0$ and oscillates as $\exp(-i\Omega t)$ in time.

(2) The transverse-electromagnetic (TEM) modes can be obtained by assuming $\{w_l(\boldsymbol{\xi},s)\}$ to be a set of Hermite-Gaussian functions of (x,y).

(3) The diffraction of an optical mode is modeled by the change of the mode function $\boldsymbol{v}_l(x,y,z,t)$ along z according to Eq. (13.16). Fresnel diffraction [27], for example, is obtained if we make the Taylor-series approximation

$$k_z(k_x,k_y,\omega) \approx \frac{\omega}{c} - \frac{k_x^2+k_y^2}{2\Omega} \tag{13.33}$$

inside the $\exp(ik_z z)$ factor in Eq. (13.16).

13.2. Incoherent light

To model incoherent light, such as the radiation from thermal or fluorescent sources, we assume a quantum state in the form

$$\boxed{\hat{\rho} = \int \Phi(\boldsymbol{\alpha}) \left|\boldsymbol{\alpha}\right\rangle \left\langle\boldsymbol{\alpha}\right| d^{2J}\boldsymbol{\alpha},} \qquad \boxed{\Phi(\boldsymbol{\alpha}) = \frac{1}{\det(\pi\Gamma)} \exp\left(-\boldsymbol{\alpha}^\dagger \Gamma^{-1} \boldsymbol{\alpha}\right),} \tag{13.34}$$

where the Sudarshan representation Φ is a zero-mean symmetric Gaussian distribution with a covariance matrix given by

$$\int \Phi(\boldsymbol{\alpha}) \alpha_l \alpha_m^* d^{2J}\boldsymbol{\alpha} = \Gamma_{lm}. \tag{13.35}$$

The word "symmetric" refers to the fact

$$\int \Phi(\boldsymbol{\alpha}) \alpha_l \alpha_m d^{2J}\boldsymbol{\alpha} = 0 \quad \forall l,m. \tag{13.36}$$

We call any state in this form a **Glauber state**. This model is motivated by the following facts:

(1) The thermal state discussed in Sec. 5.3 is a Glauber state.

(2) Under passive linear optics, an initial Glauber state would evolve to

$$\hat{\rho} = \int \Phi(\boldsymbol{\alpha}) \left|V\boldsymbol{\alpha}\right\rangle \left\langle V\boldsymbol{\alpha}\right| d^{2J}\boldsymbol{\alpha} = \int \Phi(V^\dagger\boldsymbol{\beta}) \left|\boldsymbol{\beta}\right\rangle \left\langle\boldsymbol{\beta}\right| d^{2J}\boldsymbol{\beta} \tag{13.37}$$

for some unitary matrix V, as we learned in Sec. 6.5.2. The Sudarshan representation in terms of $\boldsymbol{\beta}$ becomes

$$\Phi(V^\dagger\boldsymbol{\beta}) = \frac{1}{\det(\pi\Gamma)} \exp\left[-\boldsymbol{\beta}^\dagger (V\Gamma V^\dagger)^{-1} \boldsymbol{\beta}\right], \tag{13.38}$$

which is still zero-mean symmetric Gaussian, except that the covariance matrix has been transformed to $V\Gamma V^\dagger$. The output state hence remains a Glauber state.

(3) To model loss, we should assume that some modes are inaccessible and trace them out, as we learned in Chapter 7. If the bath is also in a Glauber state initially, then it can be shown that the state after passive linear optics and partial trace is still a Glauber state; see Exercise 13.1.

(4) The evolution of the covariance matrix in passive linear optics is consistent with the basic principles of statistical optics [28].

(5) With a Glauber state, the quadrature observables of each mode are zero-mean Gaussian random variables with the same variance. This agrees with the common assumption in statistical optics that the fields of incoherent light are zero-mean Gaussian random processes with the same variance for the quadratures of each mode.
(6) The photon-counting statistics with a Glauber state follows Mandel's formula given by Eq. (5.59), which has been verified by experiments for many common light sources.

In addition to being a decent model, Glauber states are also mathematically convenient because each is completely specified by the covariance matrix Γ, which is a $J \times J$ matrix for J modes, a much simpler mathematical object than the infinite-dimensional $\hat{\rho}$.

A classical-quantum correspondence can now be established by assuming that the **mutual coherence function** in statistical optics is given by

$$\boxed{\gamma(\boldsymbol{\xi}, s, \boldsymbol{\xi}', s') \equiv \left\langle \hat{E}_s^{(-)}(x', y', z' = 0, t') \hat{E}_{s'}^{(+)}(x, y, z = 0, t) \right\rangle,} \qquad \hat{E}_s \equiv \tilde{\boldsymbol{e}}_s^* \cdot \hat{\boldsymbol{E}}, \tag{13.39}$$

which is the covariance between the complex electric fields at two different points $\boldsymbol{\xi} = (x, y, t)$ and $\boldsymbol{\xi}' = (x', y', t')$ on a plane at $z = 0$. The mutual coherence can be related to the covariance matrix Γ in a Glauber state through the following recipe:

(1) Assuming the spatiotemporal modes in Sec. 13.1 and a coherent state that satisfies

$$\hat{f}_l \left|\boldsymbol{\alpha}\right\rangle = \alpha_l \left|\boldsymbol{\alpha}\right\rangle, \tag{13.40}$$

the covariance matrix for a Glauber state becomes

$$\Gamma_{lm} = \int \Phi(\boldsymbol{\alpha}) \alpha_l \alpha_m^* d^{2J}\boldsymbol{\alpha} = \int \Phi(\boldsymbol{\alpha}) \alpha_l \alpha_m^* d^{2J}\boldsymbol{\alpha} = \operatorname{tr} \int \Phi(\boldsymbol{\alpha}) \hat{f}_l \left|\boldsymbol{\alpha}\right\rangle \left\langle\boldsymbol{\alpha}\right| \hat{f}_m^\dagger d^{2J}\boldsymbol{\alpha} = \operatorname{tr}\left(\hat{f}_l \hat{\rho} \hat{f}_m^\dagger\right). \tag{13.41}$$

(2) Under the narrowband approximations, the mutual coherence can be related to Γ by

$$\gamma(\boldsymbol{\xi}, s, \boldsymbol{\xi}', s') = \sum_{l,m} \left[\tilde{\boldsymbol{e}}_s^* \cdot \boldsymbol{v}_l(\boldsymbol{r}, t)\right] \operatorname{tr}\left(\hat{f}_l \hat{\rho} \hat{f}_m^\dagger\right) \left[\tilde{\boldsymbol{e}}_{s'}^* \cdot \boldsymbol{v}_m(\boldsymbol{r}', t')\right]^* \qquad \text{(using Eqs. (13.13) and (13.39))} \tag{13.42}$$

$$\approx \frac{\hbar\Omega}{2\epsilon_0 c} e^{-i\Omega(t-t')} \sum_{l,m} w_l(\boldsymbol{\xi}, s) \Gamma_{lm} w_m^*(\boldsymbol{\xi}', s'). \qquad \text{(using Eqs. (13.32) and (13.41))} \tag{13.43}$$

(3) Using the orthonormal condition given by Eq. (13.31), we can also express the covariance matrix Γ in terms of the mutual coherence γ as

$$\boxed{\Gamma_{lm} = \frac{2\epsilon_0 c}{\hbar\Omega} \sum_{s,s'} \iiint \iiint w_l^*(\boldsymbol{\xi}, s) \gamma(\boldsymbol{\xi}, s, \boldsymbol{\xi}', s') w_m(\boldsymbol{\xi}', s') e^{i\Omega(t-t')} d^3\boldsymbol{\xi} d^3\boldsymbol{\xi}'.} \tag{13.44}$$

This recipe allows us to translate any result in statistical optics in terms of the mutual coherence to the quantum regime by relating it to the covariance matrix of a Glauber state, provided that the problem at hand satisfies all the assumptions made in this chapter.

Exercise 13.1.

(1) Let $\mathcal{H}_A$ be a Hilbert space for J system modes and $\mathcal{H}_B$ be a Hilbert space for K bath modes. Let $\hat{\rho}$ be a Glauber state on $\mathcal{H}_A$ with covariance matrix Γ and $\hat{\rho}_B$ be a Glauber state on $\mathcal{H}_B$ with covariance matrix $\Gamma^{(B)}$. Show that $\hat{\rho} \otimes \hat{\rho}_B$ is a Glauber state on $\mathcal{H}_A \otimes \mathcal{H}_B$ and find its covariance matrix in terms of Γ and $\Gamma^{(B)}$. You may assume that $\left|\boldsymbol{\alpha}\right\rangle = \left|\boldsymbol{\alpha}^{(A)}\right\rangle \otimes \left|\boldsymbol{\alpha}^{(B)}\right\rangle$ is a coherent state on $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\left|\boldsymbol{\alpha}^{(A)}\right\rangle$ is a coherent state in $\mathcal{H}_A$, $\left|\boldsymbol{\alpha}^{(B)}\right\rangle$ is a coherent state in $\mathcal{H}_B$, and

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}^{(A)} \oplus \boldsymbol{\alpha}^{(B)} \equiv \begin{pmatrix} \boldsymbol{\alpha}^{(A)} \\ \boldsymbol{\alpha}^{(B)} \end{pmatrix}, \tag{13.45}$$

where $\oplus$ is the direct sum (see Sec. B.11).

(2) To model loss, suppose that the system and the bath go through some passive linear optics together, modeled by a unitary $\hat{U}$ operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ and a V matrix, such that

$$\hat{U}\,|\boldsymbol{\alpha}\rangle = |V\boldsymbol{\alpha}\rangle\,, \qquad\qquad V\boldsymbol{\alpha} = \begin{pmatrix} V^{(AA)} & V^{(AB)} \\ V^{(BA)} & V^{(BB)} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}^{(A)} \\ \boldsymbol{\alpha}^{(B)} \end{pmatrix}, \tag{13.46}$$

where $V^{(AA)}$ is a $J \times J$ matrix, $V^{(AB)}$ is a $J \times K$ matrix, $V^{(BA)}$ is a $K \times J$ matrix, and $V^{(BB)}$ is a $K \times K$ matrix. Then we trace out the bath degree of freedom. Show that the resulting system state

$$\hat{\sigma} = \mathrm{tr}_B \left[\hat{U}(\hat{\rho} \otimes \hat{\rho}_B)\hat{U}^\dagger\right] \tag{13.47}$$

on $\mathcal{H}_A$ remains a Glauber state and find its covariance matrix in terms of Γ, $\Gamma^{(B)}$, and the V matrix given above.

(3) If $\hat{\rho}_B$ is the vacuum state, find its covariance matrix $\Gamma^{(B)}$ and find the covariance matrix of the final Glauber state $\hat{\sigma}$ in terms of Γ and the V matrix given above.

13.3. Spectral modes

Suppose that each $(\boldsymbol{\xi}, s)$-space amplitude $w_l(\boldsymbol{\xi}, s)$ is separable as follows:

$$w_l(\boldsymbol{\xi}, s) = w_{q,m}(\boldsymbol{\xi}, s) = \phi_q(x, y, s)\varphi_m(t), \tag{13.48}$$

where the mode label l is now defined as

$$l = (q, m) \tag{13.49}$$

in terms of the label q for the spatial/polarization mode and the label m for the temporal mode. Let the temporal amplitude $\varphi_m(t)$ over a time interval T be

$$\varphi_m(t) = \frac{1}{\sqrt{T}} \exp(-i\tilde{\omega}_m t), \quad |t| \leq \frac{T}{2}, \tag{13.50}$$

where

$$\tilde{\omega}_m = \tilde{\omega}_1 + \frac{2\pi(m-1)}{T}, \quad m = 1, \ldots, M. \tag{13.51}$$

The electric field of each mode then oscillates with frequency $\Omega + \tilde{\omega}_m$. The temporal amplitudes $\{\varphi_l(t)\}$ are orthonormal in the sense of

$$\int_{-T/2}^{T/2} \varphi_m^*(t)\varphi_{m'}(t)dt = \delta_{mm'}. \tag{13.52}$$

T is assumed to be finite to make the math more tractable, but we also assume that it is very long relative to Ω and often take the limit $T \to \infty$ if appropriate.

With incoherent light, it is often reasonable to assume

$$\Gamma_{ll'} = \Gamma_{(q,m),(q',m')} = 0 \quad \text{if } m \neq m', \tag{13.53}$$

meaning that there is no correlation between two modes if they do not have the same frequency. The thermal state, for example, obeys this condition. Moreover, most linear-optics components are time-invariant systems that do not couple modes with different frequencies, so the covariance remains zero after the light passes through such components. Another motivation is that incoherent light is often a stationary process in the sense that the mutual coherence is a function of $t - t'$ only in terms of its time dependence, so Eq. (13.44) would also imply $\Gamma_{ll'} = 0$ in the limit of $T \to \infty$ if the two modes do not have the same frequency.

With no covariance between modes with different frequencies, we can partition Γ as the direct sum

$$\Gamma = \Gamma^{(1)} \oplus \Gamma^{(2)} \oplus \cdots \oplus \Gamma^{(M)} = \begin{pmatrix} \Gamma^{(1)} & & & \\ & \Gamma^{(2)} & & \\ & & \ddots & \\ & & & \Gamma^{(M)} \end{pmatrix}, \tag{13.54}$$

where

$$\Gamma^{(m)}_{qp} \equiv \Gamma_{(q,m),(p,m)} \tag{13.55}$$

is the covariance matrix for J_m modes with the same frequency $\tilde{\omega}_m$. We also partition the complex amplitudes accordingly:

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}^{(1)} \oplus \boldsymbol{\alpha}^{(2)} \oplus \cdots \oplus \boldsymbol{\alpha}^{(M)} = \begin{pmatrix} \boldsymbol{\alpha}^{(1)} \\ \boldsymbol{\alpha}^{(2)} \\ \vdots \\ \boldsymbol{\alpha}^{(M)} \end{pmatrix}, \tag{13.56}$$

where $\boldsymbol{\alpha}^{(m)}$ is a column vector of amplitudes for the J_m modes with the same frequency $\tilde{\omega}_m$, so that the Sudarshan representation becomes

$$P(\boldsymbol{\alpha}) = \prod_{m=1}^{M} \frac{1}{\det\left(\pi\Gamma^{(m)}\right)} \exp\left(-\boldsymbol{\alpha}^{(m)\dagger}\Gamma^{(m)-1}\boldsymbol{\alpha}^{(m)}\right), \tag{13.57}$$

and the Glauber state becomes

$$\hat{\rho} = \bigotimes_{m=1}^{M} \hat{\rho}^{(m)}, \qquad \hat{\rho}^{(m)} \equiv \int \frac{1}{\det\left(\pi\Gamma^{(m)}\right)} \exp\left(-\boldsymbol{\alpha}^{(m)\dagger}\Gamma^{(m)-1}\boldsymbol{\alpha}^{(m)}\right) \left|\boldsymbol{\alpha}^{(m)}\right\rangle \left\langle\boldsymbol{\alpha}^{(m)}\right| d^{2J_m}\boldsymbol{\alpha}^{(m)}. \tag{13.58}$$

Long story short, the zero covariance between modes with different frequencies allows us to factorize the Glauber state into a tensor product of states, where each state is a Glauber state for modes with the same frequency.

13.4. Poisson approximation

We now focus on $\hat{\rho}^{(m)}$ for the spatial/polarization modes with a specific frequency $\tilde{\omega}_m$. For brevity, we write

$$\hat{f}_q = \hat{f}_{q,m}. \tag{13.59}$$

For weak sources at optical frequencies, such as astronomical sources or fluorescent particles, it is often the case that the average photon number in one spectral mode received by an imaging system is much smaller than 1. Mathematically, this means that

$$\epsilon \equiv \operatorname{tr}\Gamma^{(m)} = \sum_q \operatorname{tr}\left(\hat{f}_q^\dagger \hat{f}_q \hat{\rho}^{(m)}\right) \ll 1. \tag{13.60}$$

We can then make the approximation that $\hat{\rho}^{(m)}$ is a linear combination of $|\text{vac}\rangle\langle\text{vac}|$, $\{|\text{vac}\rangle\langle 1_q|\}$, $\{|1_q\rangle\langle\text{vac}|\}$, and $\{|1_q\rangle\langle 1_p|\}$ only, where

$$|1_q\rangle \equiv \hat{f}_q^\dagger |\text{vac}\rangle \tag{13.61}$$

is the state with one photon in spatial/polarization mode q. It can be shown that, for a Glauber state,

$$\langle\boldsymbol{n}|\,\hat{\rho}^{(m)}\left|\boldsymbol{n}'\right\rangle = 0 \quad \text{if } \sum_q n_q \neq \sum_q n'_q, \tag{13.62}$$

so we can assume

$$\hat{\rho}^{(m)} = \langle \text{vac}| \hat{\rho}^{(m)} |\text{vac}\rangle |\text{vac}\rangle \langle \text{vac}| + \sum_{q,p} \langle 1_q| \hat{\rho}^{(m)} |1_p\rangle |1_q\rangle \langle 1_p|, \tag{13.63}$$

$$\langle \text{vac}| \hat{\rho}^{(m)} |\text{vac}\rangle = \int \Phi^{(m)}(\boldsymbol{\alpha}) e^{-\|\boldsymbol{\alpha}\|^2} d^{2J_m}\boldsymbol{\alpha} = 1 - \epsilon + O(\epsilon^2), \tag{13.64}$$

$$\langle 1_q| \hat{\rho}^{(m)} |1_p\rangle = \int \Phi^{(m)}(\boldsymbol{\alpha}) e^{-\|\boldsymbol{\alpha}\|^2} \alpha_q \alpha_p^* d^{2J_m}\boldsymbol{\alpha} = \Gamma^{(m)}_{qp} + O(\epsilon^2), \tag{13.65}$$

where $O(\epsilon^2)$ denotes terms on the order of ϵ^2 or smaller, which we assume to be negligible. All other matrix entries are $O(\epsilon^2)$ and can be neglected. Hence,

$$\boxed{\hat{\rho}^{(m)} \approx (1-\epsilon) |\text{vac}\rangle \langle \text{vac}| + \hat{\Gamma}^{(m)},} \qquad \boxed{\hat{\Gamma}^{(m)} \equiv \sum_{q,p} \Gamma^{(m)}_{qp} |1_q\rangle \langle 1_p|,} \qquad \boxed{\epsilon = \operatorname{tr} \hat{\Gamma}^{(m)}.} \tag{13.66}$$

This approximation of the density operator is extremely useful in quantum information calculations [29, 30, 31].

An important consequence of Eq. (13.66) is that it gives rise to Poisson statistics for photon counting. To see this, first consider photon counting in one spectral mode. Let the photon count in mode (q, m) be $n_{q,m}$. The probability of finding no photon in one spectral mode is

$$P[n_{q,m} = 0 \text{ for all } q] = \langle \text{vac}| \hat{\rho}^{(m)} |\text{vac}\rangle = 1 - \epsilon, \tag{13.67}$$

the probability of finding one photon is

$$P\left[\sum_q n_{q,m} = 1\right] = \sum_q \langle 1_q| \hat{\rho}^{(m)} |1_q\rangle = \epsilon, \tag{13.68}$$

and given that there is one photon, the probability of finding the photon in spatial/polarization mode q is

$$P\left[n_{q,m} = 1 \middle| \sum_p n_{p,m} = 1\right] = \frac{1}{\epsilon} \langle 1_q| \hat{\rho}^{(m)} |1_q\rangle = \frac{1}{\epsilon} \Gamma^{(m)}_{qq}. \tag{13.69}$$

If we now assume that all the covariance matrices $\{\Gamma^{(m)}\}$ for different frequencies are identical and, for each spatial/polarization mode q, we integrate the photon counts $n_{q,m}$ over all the frequencies to obtain an integrated photon count

$$n_q \equiv \sum_{m=1}^{M} n_{q,m}, \tag{13.70}$$

the integrated photon counts $\{n_q\}$ in the spatial/polarization modes become Poisson in the limit of

$$\epsilon \to 0, \qquad M \to \infty, \qquad M\epsilon \text{ held fixed}, \tag{13.71}$$

according to Sec. C.7. This result is consistent with the Poisson model commonly assumed in optical astronomy [32, 33] and fluorescence microscopy [34], offering another justification of the approximation in Eq. (13.66).

Note that our derivation of the Poisson model works for photon counting with respect to any set of spatial/polarization modes, since we haven't assumed anything specific about the modes.

Side note. *The photon-counting distribution for thermal, fluorescent, or atomic sources is often not exactly Poisson, and any deviation from the Poisson model is called bunching or antibunching [35]. To model bunching or antibunching, one needs to include the multi-photon components of $\hat{\rho}^{(m)}$, i.e., the higher-order terms $\sum_{\boldsymbol{n},\boldsymbol{n}'} \langle \boldsymbol{n}| \hat{\rho}^{(m)} |\boldsymbol{n}'\rangle |\boldsymbol{n}\rangle \langle \boldsymbol{n}'|$ with $\sum_q n_q = \sum_q n'_q \geq 2$. Calculations have shown, however, that such terms are insigificant if $\epsilon \ll 1$:*

(1) In astronomy, Hanbury-Brown-Twiss interferometry, also called intensity interferometry, postselects the two-photon events in each temporal mode, and one must consider at least the two-photon components of $\rho^{(m)}$ to model it. Unfortunately, it turns out to have a terrible signal-to-noise ratio compared with ordinary stellar interferometry that relies on one-photon events [32].

(2) *Calculations in quantum information theory [36, 37, 38] also find that, when $\epsilon \ll 1$, the effect of the higher-order terms on the total amount of information in the light is negligible.*

The reason is simple: the probability of having two or more photons in each spectral mode is $O(\epsilon^2)$, which is much smaller than the one-photon probability ϵ; such rare events cannot contribute significant information on average.

13.5. Imaging

13.5.1. Randomly polarized light. First let us be more specific about the polarizations. Assume

$$w_l(\boldsymbol{\xi}, s) = w_{q,\sigma,m}(\boldsymbol{\xi}, s) = \phi_q(x, y)\delta_{s\sigma}\varphi_m(t), \tag{13.72}$$

where the mode label now consists of

$$l = (q, \sigma, m), \tag{13.73}$$

q is the label for the spatial part, $\sigma = 1, 2$ is the label for the polarization part, and m is the label for the spectral part. If the light is randomly polarized, then

$$\Gamma_{ll'} = \Gamma_{(q,\sigma,m),(q',\sigma',m')} = 0 \quad \text{if } \sigma \neq \sigma' \tag{13.74}$$

for any two modes with orthogonal polarizations, and we can once again partition the covariance matrix as

$$\Gamma = \bigoplus_{\sigma,m} \Gamma^{(\sigma,m)}, \qquad \Gamma^{(\sigma,m)}_{qp} \equiv \Gamma_{(q,\sigma,m),(p,\sigma,m)}. \tag{13.75}$$

$\Gamma^{(\sigma,m)}$ is now a covariance matrix for spatial modes with a given polarization σ and frequency $\tilde{\omega}_m$.

With all these assumptions and using Eq. (13.44), $\Gamma^{(\sigma,m)}$ can be expressed as

$$\boxed{\Gamma^{(\sigma,m)}_{qp} = \iint\!\!\iint \phi^*_q(x, y)\gamma^{(\sigma,m)}(x, y, x', y')\phi_p(x', y')dxdydx'dy',} \tag{13.76}$$

where

$$\gamma^{(\sigma,m)}(x, y, x', y') \equiv \frac{2\epsilon_0 c}{\hbar\Omega}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \varphi^*_m(t)\varphi^*_m(t')\gamma(\boldsymbol{\xi}, \sigma, \boldsymbol{\xi}', \sigma)e^{i\Omega(t-t')}dtdt' \tag{13.77}$$

is the spatial part of the mutual coherence. Using the same Poisson approximation in Sec. 13.4, we can write

$$\hat{\rho} = \bigotimes_{\sigma,m} \hat{\rho}^{(\sigma,m)}, \qquad \hat{\rho}^{(\sigma,m)} = (1 - \operatorname{tr}\hat{\Gamma}^{(\sigma,m)})\,|\text{vac}\rangle\langle\text{vac}| + \hat{\Gamma}^{(\sigma,m)}, \qquad \hat{\Gamma}^{(\sigma,m)} = \sum_{q,p} \Gamma^{(\sigma,m)}_{qp}\,|1_q\rangle\langle 1_p|\,. \tag{13.78}$$

Our remaining task is to find $\hat{\Gamma}^{(\sigma,m)}$.

13.5.2. Statistical optics. Let us now review the key results in statistical optics [32] with criminal brevity. A point source excites a spatially localized mode near (u, v) on the object plane. The mode turns into a spherical wave as it propagates away from the source. A diffraction-limited optical system collects part of it through an aperture and passes the light to a detection plane. The mutual coherence on the detection plane becomes [32]

$$\gamma^{(\sigma,m)}(x, y, x', y') \propto I\psi(x, y|u, v)\psi^*(x', y'|u, v), \tag{13.79}$$

where I is the intensity of the source and ψ is the **point-spread function** of the system for the optical field. For example,

(1) if the detection plane is right at the aperture (called the pupil plane) before any lenses, then $\psi(x, y|u, v)$ is simply the spherical-wave solution,

(2) if the detection plane is an image plane, then $\psi(x, y|u, v)$ can be modeled as a function of $(x - u, y - v)$.

With multiple incoherent point sources at object-plane positions $\{(u_p, v_p)\}$ and with intensities $\{I_p\}$, there is no correlation between the fields due to different sources, and the mutual coherence is the sum

$$\gamma^{(\sigma,m)}(x, y, x', y') \propto \sum_p I_p\psi(x, y|u_p, v_p)\psi^*(x', y'|u_p, v_p). \tag{13.80}$$

More generally, we can regard an arbitrary number of incoherent point sources as one spatially incoherent extended object with intensity function $I(u,v)$ on the object plane, so that the mutual coherence on the detection plane becomes

$$\boxed{\gamma^{(\sigma,m)}(x,y,x',y') \propto \iint I(u,v)\psi(x,y|u,v)\psi^*(x',y'|u,v)dudv.} \tag{13.81}$$

The setup is illustrated in Fig. 13.3. The famous Van Cittert-Zernike theorem in statistical optics (https://en.wikipedia.org/wiki/Van_Cittert%E2%80%93Zernike_theorem) is an example of Eq. (13.81) if we take the detection plane to be the pupil plane and ψ to be the spherical wave.

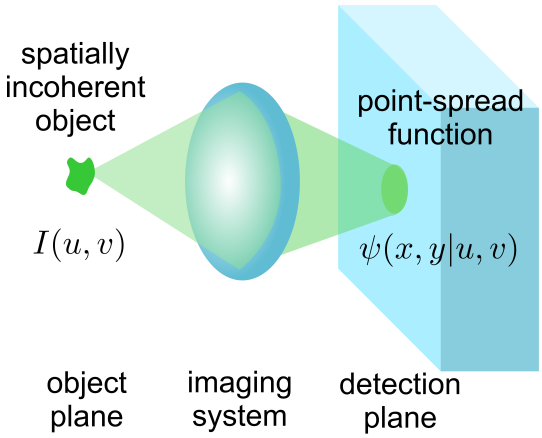

FIGURE 13.3. A diffraction-limited imaging system.

13.5.3. Classical-quantum correspondence. To relate the mutual coherence $\gamma^{(\sigma,m)}$ to the covariance matrix $\Gamma^{(\sigma,m)}$ in a Glauber state, use Eq. (13.28) to write the spatial-mode annihilation operator as

$$\hat{f}_q = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_q^*(x,y)\hat{d}(x,y)dxdy, \tag{13.82}$$

where $\hat{d}(x,y)$ is related to the $\hat{c}$ operator in Eq. (13.29) by

$$\hat{d}(x,y) \equiv \int_{-\infty}^{\infty} \varphi_m^*(t)\hat{c}(\boldsymbol{\xi},\sigma)dt, \qquad \left[\hat{d}(x,y),\hat{d}^\dagger(x',y')\right] = \delta(x-x')\delta(y-y'). \tag{13.83}$$

Define also

$$|\psi_{u,v}\rangle \equiv \left[\iint \psi(x,y|u,v)\hat{d}^\dagger(x,y)dxdy\right]|\text{vac}\rangle \tag{13.84}$$

as the state of a detection-plane photon emitted by a point source at object-plane position (u,v), assuming that the point-spread function is normalized as

$$\langle\psi_{u,v}|\psi_{u,v}\rangle = \iint |\psi(x,y|u,v)|^2 dxdy = 1. \tag{13.85}$$

Then

$$\langle 1_q|\psi_{u,v}\rangle = \iint \phi_q^*(x,y)\psi(x,y|u,v)dxdy, \tag{13.86}$$

and this inner product can now be combined with Eqs. (13.76) and (13.81) to give

$$\Gamma_{qp}^{(\sigma,m)} \propto \iint I(u,v)\,\langle 1_q|\psi_{u,v}\rangle\,\langle\psi_{u,v}|1_p\rangle\,dudv, \tag{13.87}$$

$$\boxed{\hat{\Gamma}^{(\sigma,m)} \propto \iint I(u,v)\,|\psi_{u,v}\rangle\,\langle\psi_{u,v}|\,dudv.} \tag{13.88}$$

Eqs. (13.78) and (13.88) are the starting point of many calculations regarding incoherent imaging in quantum information theory [29, 30, 31].

APPENDIX A

Blackbody Radiation*

A.1. Rayleigh-Jeans

Consider a box with some matter that can both absorb and emit EM radiation, such as the wall of an oven or atoms inside a star. We call the matter blackbody because it can absorb light at all frequencies, but in practice anything can absorb and emit light. We focus on the EM fields and assume that the blackbody is the "heat bath." According to Gibbs, when the fields and the blackbody are in a thermal equilibrium, each degree of freedom of the fields should have a probability density of energy given by

$$f(E) = \frac{\exp(-\beta E)}{\int_0^\infty \exp(-\beta E')dE'}, \qquad \beta \equiv \frac{1}{k_B T}, \tag{A.1}$$

where k_B is called the Boltzmann constant (even though it was first proposed by Planck) and T is the temperature. Each degree of freedom is a mode of the EM fields inside the box. The average energy of each mode is then

$$\bar{E} = \int_0^\infty E f(E) dE = \frac{1}{\beta} = k_B T. \tag{A.2}$$

This result is consistent with the equipartition theorem for harmonic oscillators. Now we define a spectral density function $S(\omega)$ as a function of the angular frequency ω as follows:

$$\boxed{\int_0^\Omega S(\omega)d\omega = \frac{\text{energy in all modes with frequencies up to } \Omega}{\text{volume of box}}.} \tag{A.3}$$

In other words, $\int_0^\Omega S(\omega)d\omega$ is the EM energy density if we include only modes with frequencies up to Ω.

For EM fields, that means we need to sum up the energies of all the modes with frequencies up to Ω to compute this integral.

Since $\bar{E}$ here is the same for all modes, we just need to count the number of modes and multiply that by $\bar{E}$. Recall

$$k_x = \frac{2\pi n_x}{L}, \qquad k_y = \frac{2\pi n_y}{L}, \qquad k_z = \frac{2\pi n_z}{L}, \qquad n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots, \tag{A.4}$$

and if we mark each possible value of (k_x, k_y, k_z) by a dot in $\boldsymbol{k}$ space, we'd get something like Fig. A.1.

(1) Each dot is separated from an adjacent dot by $2\pi/L$, and we have a **lattice** of dots in general.
(2) Remember also that, for each value of $\boldsymbol{k}$, we have two polarizations, so each dot denotes two polarization modes.
(3) Recall that each mode has frequency

$$\omega(\boldsymbol{k}) = c|\boldsymbol{k}|, \tag{A.5}$$

so the modes with $\omega(\boldsymbol{k}) = c|\boldsymbol{k}| \le \Omega$ would be the modes inside a sphere in $\boldsymbol{k}$ space with radius $|\boldsymbol{k}| \le \Omega/c$.

To simplify the counting, we introduce the concept of **mode density** $\rho(\boldsymbol{k})$:

$$\iiint_{\mathcal{V}} \rho(\boldsymbol{k}) d^3\boldsymbol{k} = \text{number of modes inside a } \boldsymbol{k}\text{-space region } \mathcal{V}. \tag{A.6}$$

Let's assume that L is very large, so that the dots are very close to each other and there are a large number of dots inside the sphere. Then we may approximate the density of the dots as a constant, i.e., assume that $\rho(\boldsymbol{k})$ is a constant.

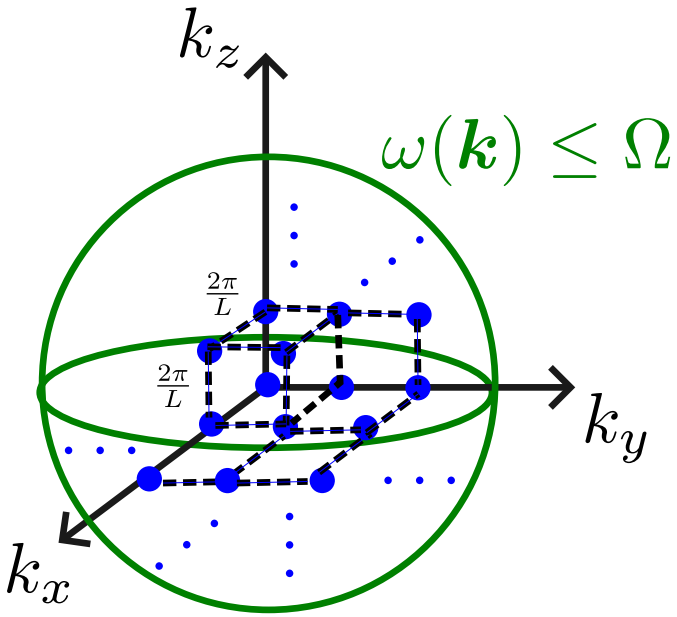

FIGURE A.1. Possible values of wavevector $\boldsymbol{k}$ for sinusoidal modes in a box. Each dot denotes two polarization modes.

There is one dot per $\boldsymbol{k}$-space volume $(2\pi/L)^3$, and there are two modes per dot, so the mode density is

$$\rho(\boldsymbol{k}) \approx \frac{2}{(2\pi/L)^3}. \tag{A.7}$$

Now the number of modes with $\omega(\boldsymbol{k}) \leq \Omega$ is simply an integration of $\rho(\boldsymbol{k})$ over the sphere with radius Ω/c in $\boldsymbol{k}$ space. Since $\rho(\boldsymbol{k})$ is a constant, the integral is simple:

$$\text{number of modes with } \omega(\boldsymbol{k}) \leq \Omega \approx \rho(\boldsymbol{k}) \times \text{volume of sphere} = \frac{2}{(2\pi/L)^3}\frac{4\pi(\Omega/c)^3}{3}. \tag{A.8}$$

Side note. *The concept of mode density and the formalism here are closely related to the important concept of* ***density of states*** *in solid-state physics.*

Putting everything together,

$$\int_0^\Omega S(\omega)d\omega = \frac{\text{average energy per mode} \times \text{number of modes with frequencies up to } \Omega}{\text{volume of box}} \tag{A.9}$$

$$= \frac{\bar{E}}{L^3} \times \frac{2}{(2\pi/L)^3}\frac{4\pi(\Omega/c)^3}{3}. \tag{A.10}$$

Differentiating both sides with respect to Ω, we obtain

$$S(\omega) = \bar{E}\frac{\omega^2}{\pi^2 c^3}. \tag{A.11}$$

We could do more physics to derive the power spectral density of the light that comes out if we poke a hole on the wall, but we wouldn't bother for now. (It has the same dependence on ω as $S(\omega)$; see Sec. A.3.) Plugging the classical prediction $\bar{E} = k_B T$ into the formula, we obtain the Rayleigh-Jeans law

$$\boxed{S_{\text{Rayleigh-Jeans}}(\omega) = \frac{\omega^2}{\pi^2 c^3}k_B T.} \tag{A.12}$$

This fits the experimental result for low ω only. The discrepancy between Rayleigh-Jeans and experiments at high frequencies is called the ultraviolet catastrophe.

A.2. Planck

Planck assumes that the energy in each mode is discrete. According to Gibbs, if the energy is discrete, the probability mass function of the energy in mode $j = (\boldsymbol{k}, s)$ should be

$$P_j(E) = \frac{\exp\left(-\beta E/\hbar\omega_j\right)}{\sum_{E'} \exp\left(-\beta E'/\hbar\omega_j\right)}, \qquad \frac{E}{\hbar\omega_j} = 0, 1, 2, \dots \tag{A.13}$$

The average energy is then

$$\bar{E}_j = \sum_E E P_j(E) = \frac{\hbar\omega_j}{\exp(\hbar\omega_j/k_BT) - 1}. \tag{A.14}$$

When $\hbar\omega_j \ll k_BT$, we have $\bar{E}_j \approx k_BT$, which agrees with the classical case, but when the frequency ω_j is high $\bar{E}_j$ becomes very different. Since the energy of each mode depends on ω_j, which depends on $\boldsymbol{k}$, we have to modify the formula for $\int_0^\Omega S(\omega)d\omega$ a bit:

$$\int_0^\Omega S(\omega)d\omega = \frac{1}{L^3} \iiint_{\mathcal{V}} \bar{E}_j \rho(\boldsymbol{k}) d^3\boldsymbol{k}. \tag{A.15}$$

In other words, we think of $\rho(\boldsymbol{k})d^3\boldsymbol{k}$ as the number of modes in a tiny region near $\boldsymbol{k}$ in $\boldsymbol{k}$ space, $\bar{E}_j$ as the energy of those modes, and the integration in $\boldsymbol{k}$ space is just a sum over all the energies in the modes inside the $\boldsymbol{k}$-space region $\mathcal{V}$. Since $\bar{E}_j$ depends only on the magnitude k of $\boldsymbol{k}$ and $\rho(\boldsymbol{k})$ is constant, it is convenient to rewrite the 3D $\boldsymbol{k}$-space integral in spherical coordinates:

$$\int_0^\Omega S(\omega)d\omega = \frac{1}{L^3} \iiint_{\mathcal{V}} \bar{E}_j \rho(\boldsymbol{k}) d^3\boldsymbol{k} = \int_0^{\Omega/c} \int_0^\pi \int_0^{2\pi} \bar{E}_j \frac{2}{(2\pi)^3} k^2 \sin\theta dk d\theta d\phi \tag{A.16}$$

$$= 4\pi \frac{2}{(2\pi)^3} \int_0^{\Omega/c} \bar{E}_j k^2 dk. \tag{A.17}$$

$$= 4\pi \frac{2}{(2\pi)^3} \frac{1}{c^3} \int_0^\Omega \bar{E}_j \omega^2 d\omega. \tag{A.18}$$

Differentiating both sides with respect to Ω, we obtain

$$\boxed{S(\omega) = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{\exp(\hbar\omega/k_BT) - 1}.} \tag{A.19}$$

This is the law Planck derived in 1900. If $\hbar\omega \ll k_BT$, the Rayleigh-Jeans law given by Eq. (A.12) is a good approximation, but otherwise Planck's law is much more accurate for high ω. Moreover, the total energy $\int_0^\infty S(\omega)d\omega$ is now finite:

$$\int_0^\infty S(\omega)d\omega = \frac{\pi^2}{15(\hbar c)^3} (k_BT)^4 \propto T^4. \tag{A.20}$$

This T^4 dependence is called the Stefan-Boltzmann law.

A.3. Spectral radiance

To convert $S(\omega)$, which is the energy spectral density inside the box, to the power spectral density you observe outside the box, imagine that there is a hole on the wall of the box where the light leaks out, or consider the light that leaks out from the surface of a star. This leakage is usually very weak relative to the total energy of the EM fields and the matter (e.g., the light leaking out an oven or light from a star is very weak relative to all the energy inside them), so it does little harm to our assumption of a thermal equilibrium between the EM fields and the matter.

Suppose that the area of the leakage is A (e.g., area of the hole or surface area of the star), and we look at the energy leaking out in one small time interval Δt. With many modes inside the box and the EM waves having

random phases, it is a good assumption that the EM energy density is going to be quite constant inside the box. The speed at which the EM energy leaks out is c. Then we can define a power spectral density $R(\omega)$ by

$$\int_0^\Omega R(\omega)d\omega = \text{power density} = \frac{\text{energy density} \times \text{volume of EM energy that leaks out}}{\Delta t} \tag{A.21}$$

$$= \left[\int_0^\Omega S(\omega)d\omega\right]\frac{A \times c\Delta t}{\Delta t} = Ac\int_0^\Omega S(\omega)d\omega, \tag{A.22}$$

$$R(\omega) = AcS(\omega). \tag{A.23}$$

We could also define an intensity spectral density $I(\omega)$ by dividing both sides by the leakage area A:

$$I(\omega) \equiv \frac{R(\omega)}{A} = cS(\omega). \tag{A.24}$$

If we look at the leaked radiation from very far away, it's going to spread evenly in all angular directions. If my detector can only detect a certain solid angle, then the detected intensity spectral density normalized by the solid angle is

$$\eta(\omega) \equiv \frac{I(\omega)}{4\pi} = \frac{c}{4\pi}S(\omega), \tag{A.25}$$

so that, given a certain solid angle that my detector can cover, the intensity spectral density is $\eta(\omega) \times$ solid angle, and if I can detect the whole 4π solid angle, then I get back $\eta(\omega)4\pi = I(\omega)$.

To obtain the exact Planck's law on Wikipedia, we need to do one final thing: convert this spectral density in terms of angular frequency ω to a spectral density $\tilde{\eta}(\nu)$ in terms of frequency $\nu = \omega/(2\pi)$ in Hertz. The two densities are related by

$$\int_0^\nu \tilde{\eta}(\nu')d\nu' = \int_0^{2\pi\nu} \eta(\omega)d\omega. \tag{A.26}$$

Differentiating with respect to ν and writing $h = 2\pi\hbar$, we finally obtain

$$\boxed{\tilde{\eta}(\nu) = 2\pi\eta(2\pi\nu) = \frac{c}{2}S(2\pi\nu) = \frac{2\nu^2}{c^2}\frac{h\nu}{\exp(h\nu/k_BT) - 1}.} \tag{A.27}$$

$\tilde{\eta}(\nu)$ is called the spectral radiance (power (Watt) per frequency (Hertz) per area (m^2) per solid angle) on Wikipedia and we've finally arrived at the exact formula.

APPENDIX B

Hilbert Spaces and the Bra-Ket Notation

B.1. Motivation for an abstract formalism

Modern physics has found it simpler and more elegant to describe objects in the physical world using **abstract mathematical concepts** beyond numbers, matrices, and functions. The most common example in classical physics is the use of **abstract vectors** to describe positions, velocities, forces, fields, etc. A vector in three dimensions is written as

$$\boldsymbol{v} = v_x\tilde{\boldsymbol{x}} + v_y\tilde{\boldsymbol{y}} + v_z\tilde{\boldsymbol{z}}. \tag{B.1}$$

$\{\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}, \tilde{\boldsymbol{z}}\}$ are unit vectors that point in three orthogonal directions, called an orthonormal basis of the vector space. v_x, v_y, and v_z are the components of the vectors along those directions in a Cartesian coordinate system. $\tilde{\boldsymbol{x}}$, $\tilde{\boldsymbol{y}}$, $\tilde{\boldsymbol{z}}$, and $\boldsymbol{v}$ are abstract objects that we call vectors to represent physical concepts; they are not numbers but something more abstract. We deal with these abstract objects by mathematically defining an **algebra** on the vectors, such as addition of two vectors $\boldsymbol{v} + \boldsymbol{w}$, multiplication of a vector by a scalar $c\boldsymbol{v}$, the dot product $\boldsymbol{v} \cdot \boldsymbol{w}$, the cross product $\boldsymbol{v} \times \boldsymbol{w}$, and some tensors to map one vector to another vector. The algebra is a set of rules about how to manipulate these abstract objects and it turns out that each operation is useful and meaningful in physics.

One simple example is the work done by a constant force $\boldsymbol{F}$ on an object moving along a straight path from initial position $\boldsymbol{r}_1$ to final position $\boldsymbol{r}_2$:

$$W = \boldsymbol{F} \cdot (\boldsymbol{r}_2 - \boldsymbol{r}_1). \tag{B.2}$$

$\boldsymbol{F}$, $\boldsymbol{r}_2$, $\boldsymbol{r}_1$ are all abstract vectors. Writing a physical law this way is obviously simpler; otherwise we'd have to write out all the components of $\boldsymbol{F}$, $\boldsymbol{r}_1$, and $\boldsymbol{r}_2$. There's also a deeper message contained in the abstract formalism: It tells us that the work done is the same regardless of how we align the basis vectors $\{\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}, \tilde{\boldsymbol{z}}\}$ in our physical problem, or where we define the origin of the Cartesian coordinate system for our position vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. In other words, some symmetry of the physics is built into the abstract formalism.

For another example, consider the vector fields, the divergence $\nabla\cdot$, and the curl $\nabla\times$ in vector calculus. They allow us to simplify Maxwell's equations from the original 20-plus equations written down by Maxwell to just four, and the equations work regardless of how we align the Cartesian coordinate system in our problem.

We have an even higher level of abstraction in advanced quantum mechanics: instead of writing the fundamental equations in terms of differential equations or matrix algebra, we write them in terms of **abstract Hilbert-space vectors** and **operators on those abstract vectors**. We treat the wavefunctions, the matrices, and the derivatives in kindergarten quantum mechanics as mere **representations** of the abstract quantities. The main reason for the abstract formalism is simplicity: the notation would be a lot more cumbersome if we used anything else. The inherent symmetry built into the abstract Hilbert-space formalism is a deeper concept that we won't touch here.

B.2. Vectors

Quantum mechanics is modeled by vectors in complex Hilbert spaces. A complex Hilbert space, commonly denoted by the caligraphic $\mathcal{H}$, is a set of elements that we call **vectors**. In the bra-ket notation, we denote each vector by a **ket** written as $|\psi\rangle$. The most important example is the state of a quantum system: we use a vector $|\psi\rangle$ to model the state at one time, and all the properties of the quantum system at that time can be derived from $|\psi\rangle$.

In mathematics, we say that a set of objects are vectors when we can do the following things with them:

(1) **Scalar multiplication**: Given a vector $|\psi\rangle$, $z\,|\psi\rangle$ is also a vector, where $z \in \mathbb{C}$ is **any complex number**. (A complex number is also called a scalar in physics, to distinguish it from vectors.)

(2) **Addition**: Given two vectors $|\psi\rangle$ and $|\phi\rangle$, their addition $|\psi\rangle + |\phi\rangle$ is also a vector.

Moreover, these operations have the following properties: For arbitrary vectors $|\psi\rangle, |\phi\rangle, |\xi\rangle$ and arbitrary complex numbers $z, w \in \mathbb{C}$,

$$|\psi\rangle + |\phi\rangle = |\phi\rangle + |\psi\rangle, \tag{B.3}$$

$$(|\psi\rangle + |\phi\rangle) + |\xi\rangle = |\psi\rangle + (|\phi\rangle + |\xi\rangle), \tag{B.4}$$

$$zw\,|\psi\rangle = (zw)\,|\psi\rangle, \tag{B.5}$$

$$(z+w)\,|\psi\rangle = z\,|\psi\rangle + w\,|\psi\rangle, \tag{B.6}$$

$$z(|\psi\rangle + |\phi\rangle) = z\,|\psi\rangle + z\,|\phi\rangle, \tag{B.7}$$

$$1\,|\psi\rangle = |\psi\rangle. \tag{B.8}$$

When we take a bunch of vectors and apply scalar multiplications and vector additions repeatedly, i.e.,

$$z_1\,|\psi_1\rangle + z_2\,|\psi_2\rangle + \dots \tag{B.9}$$

we say that this is a **linear combination** of the vectors $\{|\psi_1\rangle, |\psi_2\rangle, \dots\}$. In physics, we also call it a **superposition**. The set of **all** possible linear combinations of a bunch of vectors is called a vector space. A Hilbert space is a special example of a vector space, and we call it complex when complex coefficients $\{z_1, z_2, \dots\}$ are allowed in a linear combination.

Because we can multiply a vector by any complex number for a complex Hilbert space, unfortunately it is impossible to draw these vectors in simple pictures, and we have to rely on algebra.

There is a special vector called the zero vector, denoted by 0 (without the $|\rangle$ for brevity). It is defined by

$$0 + |\psi\rangle = |\psi\rangle \quad \forall\, |\psi\rangle \in \mathcal{H}. \tag{B.10}$$

Think of it as a vector with zero length.

Almost any Hilbert space that we encounter in physics can be expressed in terms of a special countable set of vectors $\{|e_1\rangle, |e_2\rangle, \dots, |e_N\rangle\}$ called a **basis** of the Hilbert space. This set is called a basis because any element of the Hilbert space can be expressed as a linear combination of the vectors in the basis, so we can write

$$|\psi\rangle = \psi_1\,|e_1\rangle + \psi_2\,|e_2\rangle + \dots + \psi_N\,|e_N\rangle \tag{B.11}$$

for some complex numbers $\psi_1, \psi_2, \dots, \psi_N$ for any $|\psi\rangle \in \mathcal{H}$. (A basis plays the same role as the unit vectors $\{\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}, \tilde{\boldsymbol{z}}\}$ you learned in high-school physics, except that now we may have a large number of dimensions, not just three.) We call $\{\psi_1, \psi_2, \dots, \psi_N\}$ the **components** of $|\psi\rangle$ with respect to the basis. A basis is also required to be linearly independent, such that the components $\{\psi_n\}$ for a given $|\psi\rangle \in \mathcal{H}$ are unique, i.e., no other set of complex numbers can satisfy Eq. (B.11) for a given $|\psi\rangle$.

Note that, given a Hilbert space, there are usually infinitely many bases that we can choose from, so we can write a vector as

$$|\psi\rangle = \psi_1\,|e_1\rangle + \psi_2\,|e_2\rangle + \dots + \psi_N\,|e_N\rangle \tag{B.12}$$

$$= \psi'_1\,|e'_1\rangle + \psi_2\,|e'_2\rangle + \dots + \psi'_N\,|e'_N\rangle \tag{B.13}$$

using another basis $\{|e'_1\rangle, \dots, |e'_N\rangle\}$ of the same Hilbert space. **For a given vector, the components depend on the chosen basis. If we choose a different basis, the components change.**

In quantum mechanics, if $|\psi\rangle$ is the state of a quantum system, then we say that ψ_n as a function of n is a **wavefunction** of the system. The wavefunction depends on the basis we choose.

B.3. Inner product

At the end of the day, we need to extract numbers from these abstract vectors to compare with experiments, and the inner product is the main mathematical way of obtaining numbers from the abstract Hilbert-space vectors.

For vectors in a Hilbert space, we can take the inner product between two vectors $|\phi\rangle$ and $|\psi\rangle$, denoted as $\langle\phi|\psi\rangle$ in the bra-ket notation. (Mathematicians don't like this notation and prefer to write it as (ϕ, ψ) or $\langle\phi, \psi\rangle$). The inner product generalizes the dot product in high-school physics. Just like the dot product, the inner product $\langle\psi|\psi\rangle$ of a

vector $|\psi\rangle$ with itself is always a nonnegative real number and we say that $\sqrt{\langle\psi|\psi\rangle}$ is the **norm** of $|\psi\rangle$ (a fancy word for length). The new feature of the inner product is that $\langle\phi|\psi\rangle$ between two different vectors is a **complex number** in general.

An inner product is defined by the following properties: For arbitrary vectors $|\psi\rangle, |\phi\rangle, |\eta\rangle$ and arbitrary complex numbers $z, w \in \mathbb{C}$,

(1) $\langle\phi|\psi\rangle$ is a complex number.
(2) If we switch the order of the two vectors, the inner product becomes the complex conjugate:

$$\boxed{\langle\phi|\psi\rangle = (\langle\psi|\phi\rangle)^*.} \tag{B.14}$$

(3) The inner product of a vector with itself is always real and nonnegative:

$$\boxed{\langle\psi|\psi\rangle \geq 0.} \tag{B.15}$$

(4) Linearity with respect to the second vector:

$$\boxed{\langle\phi|\left(z|\psi\rangle + w|\eta\rangle\right) = z\langle\phi|\psi\rangle + w\langle\phi|\eta\rangle.} \tag{B.16}$$

(5) $\langle\psi|\psi\rangle = 0$ if and only if $|\psi\rangle = 0$ (the zero vector). In other words, the zero vector is the unique vector that has zero length $\sqrt{\langle\psi|\psi\rangle} = 0$.

To compute the inner product in practice, we assume that the Hilbert space has an **orthonormal basis** $\{|e_1\rangle, |e_2\rangle, \ldots, |e_N\rangle\}$, obeying

$$\langle e_n|e_m\rangle = \delta_{nm} \equiv \begin{cases} 1, & n = m, \\ 0, & n \neq m, \end{cases} \tag{B.17}$$

where δ_{nm} is called the Kronecker delta and $\equiv$ means "defined as." In other words, each vector in the basis has **unit norm**

$$\sqrt{\langle e_n|e_n\rangle} = 1 \tag{B.18}$$

and is **orthogonal** to all the other vectors:

$$\langle e_n|e_m\rangle = 0 \text{ if } n \neq m. \tag{B.19}$$

Given an orthonormal basis, we can express each vector in terms of the components

$$|\phi\rangle = \sum_n \phi_n |e_n\rangle = \phi_1|e_1\rangle + \cdots + \phi_N|e_N\rangle, \tag{B.20}$$

$$|\psi\rangle = \sum_n \psi_n |e_n\rangle = \psi_1|e_1\rangle + \cdots + \psi_N|e_N\rangle. \tag{B.21}$$

Then their inner product is given by the following recipe:

$$\boxed{\langle\phi|\psi\rangle = \sum_n \phi_n^*\psi_n = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \cdots + \phi_N^*\psi_N.} \tag{B.22}$$

Two important points to remember about the recipe:

(1) The inner product is like the dot product, except that we must remember to take the **complex conjugate** of the components of the first vector. If the components are all real then the inner product becomes the same as the dot product.
(2) We must pick the **same basis** for the two vectors and the basis must be **orthonormal**, otherwise the recipe doesn't work.

Remark B.1.

(1) *Orthogonal is just a fancy word for perpendicular—two vectors are said to be orthogonal if their inner product is zero. "Orthonormal" means orthogonal and normalized—a vector is called normalized if its norm is equal to 1.*
(2) *The unit vectors $\{\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}, \tilde{\boldsymbol{z}}\}$ in high-school physics are an example of an orthonormal basis of a 3D vector space.*
(3) *The number of vectors N in an orthonormal basis is called the **dimension** of the Hilbert space.*

Another way of writing the inner product is to write the components of each vector as a **column vector**:

$$\boldsymbol{\psi} \equiv \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}, \qquad \boldsymbol{\phi} \equiv \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_N \end{pmatrix}. \tag{B.23}$$

We call $\boldsymbol{\psi}$ a **column-vector representation** of $|\psi\rangle$. Again, the representation depends on the chosen basis. Then the inner product can be written in terms of matrix algebra as

$$\boxed{\langle\phi|\psi\rangle = \boldsymbol{\phi}^\dagger\boldsymbol{\psi} = \begin{pmatrix} \phi_1^* & \dots & \phi_N^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix},} \tag{B.24}$$

where † is the **conjugate transpose**.

Exercise B.1. If

$$|\phi\rangle = z\,|\phi_1\rangle + w\,|\phi_2\rangle\,, \tag{B.25}$$

show that

$$\boxed{\langle\phi|\psi\rangle = z^*\,\langle\phi_1|\psi\rangle + w^*\,\langle\phi_2|\psi\rangle\,.} \tag{B.26}$$

We say that the inner product is **antilinear with respect to the first vector**.

With the inner product, we can finally say what a Hilbert space $\mathcal{H}$ is:

(1) It is a vector space—the set of *all* linear combinations of the vectors in a basis as per Eq. (B.11).
(2) An inner product between any two vectors in the Hilbert space is defined.

The precise mathematical definition is a bit more complicated but not very important in physics. In physics, we are blessed by the existence of orthonormal bases, so calculations are nothing more than matrix algebra, e.g., Eq. (B.24), in a fancy language.

Exercise B.2. Let $\{|0\rangle\,, |1\rangle\}$ be an orthonormal basis. Compute $\langle\phi|\psi\rangle$, $\langle\psi|\psi\rangle$ and $\langle\phi|\phi\rangle$ if

(1)
$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \qquad |\phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \tag{B.27}$$

(2)
$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i\,|1\rangle), \qquad |\phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i\,|1\rangle). \tag{B.28}$$

(3)
$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i\,|1\rangle), \qquad |\phi\rangle = \frac{1}{\sqrt{2}}(-i\,|0\rangle + |1\rangle). \tag{B.29}$$

Exercise B.3. Prove that, given an orthonormal basis $\{|e_n\rangle\}$, each component ψ_n in the expansion of a vector $|\psi\rangle$ given by Eq. (B.11) can be obtained from the formula

$$\boxed{\psi_n = \langle e_n|\psi\rangle\,.} \tag{B.30}$$

Exercise B.4. Given one orthonormal basis $\{|e_n\rangle : n = 1, \ldots, N\}$, show that the basis consisting of

$$\left|e'_n\right\rangle = \sum_{m=1}^{N} U_{nm} \left|e_m\right\rangle \quad n = 1, \ldots, N, \tag{B.31}$$

where U is a unitary matrix, is another orthonormal basis. Show that the converse is also true: if $\{|e_n\rangle\}$ and $\{|e'_n\rangle\}$ are orthonormal bases of a Hilbert space, then they must be related by some unitary matrix as per Eq. (B.31). Find the relations between the components $\{\langle e_n|\psi\rangle\}$ with respect to the original basis and the components $\{\langle e'_n|\psi\rangle\}$ with respect to the new basis.

Exercise B.5. Show that the inner product is given by Eq. (B.22) regardless of the orthonormal basis we pick to define the components.

Exercise B.6. Suppose that there is just one element $|e_1\rangle$ in an orthonormal basis of a Hilbert space. How many vectors in total are there in the Hilbert space? If there are N elements in an orthonormal basis, how many vectors in total are there in the Hilbert space?

Exercise B.7. How would you define a 0-dimensional Hilbert space?

B.4. Operators

An operator maps a vector to another vector. In kindergarten quantum mechanics, we usually put a hat on it (like this: $\hat{A}$) to distinguish it from a scalar, but note that research papers and a lot of books often don't do that. If $\hat{A}$ maps a vector in $\mathcal{H}$ to another vector in the same space $\mathcal{H}$, we say that $\hat{A}$ is an operator **on** $\mathcal{H}$.

All operators considered in this book are linear, in the sense that

$$\boxed{\hat{A}(z\left|\psi\right\rangle + w\left|\phi\right\rangle) = z\hat{A}\left|\psi\right\rangle + w\hat{A}\left|\phi\right\rangle,} \tag{B.32}$$

for any $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ and any $z, w \in \mathbb{C}$. In other words, we can always pull an operator inside a sum, and pull any scalar outside an operator.

Assume an orthonormal basis $\{|e_n\rangle\}$. The most powerful notation in the bra-ket formalism is the **ket-bra** form of an operator:

$$\boxed{\hat{A} = \sum_{n,m} A_{nm} \left|e_n\right\rangle \left\langle e_m\right|,} \tag{B.33}$$

where each A_{nm} is a complex number, and A is a matrix called a **matrix representation** of $\hat{A}$, or simply a matrix of $\hat{A}$. Note that the matrix depends on the chosen basis. Notice that we write a ket first and a bra second in this ket-bra form, and it is a double sum. When we apply an operator in this form to a ket $|\psi\rangle$, we obtain

$$\hat{A}\left|\psi\right\rangle = \sum_{n,m} A_{nm} \left|e_n\right\rangle \left\langle e_m|\psi\right\rangle. \tag{B.34}$$

This equation involves the following steps:

(1) Take the inner product of $|\psi\rangle$ with $|e_m\rangle$ to obtain the components $\langle e_m|\psi\rangle$ of $|\psi\rangle$.
(2) Multiply the components with the A matrix to obtain $\sum_m A_{nm} \langle e_m|\psi\rangle$, which is a set of complex numbers.
(3) Use the complex numbers from the previous step to compute the linear combination

$$\hat{A}\left|\psi\right\rangle = \sum_{n} \left(\sum_{m} A_{nm} \left\langle e_m|\psi\right\rangle \right) \left|e_n\right\rangle. \tag{B.35}$$

The result is a linear combination of kets, so it is also a vector.

The second step above is equivalent to **matrix algebra**. If we want to compute the components $\langle e_n| \hat{A} |\psi\rangle$ of the output vector directly, we can write

$$\langle e_n| \hat{A} |\psi\rangle = \langle e_n| \sum_{j,m} A_{jm} |e_j\rangle \langle e_m|\psi\rangle \tag{B.36}$$

$$= \sum_{j,m} A_{jm} \langle e_n|e_j\rangle \langle e_m|\psi\rangle \qquad \text{(linearity of inner product)} \tag{B.37}$$

$$= \sum_{j,m} A_{jm}\delta_{nj} \langle e_m|\psi\rangle \qquad (\{|e_n\rangle\} \text{ are orthonormal}) \tag{B.38}$$

$$= \sum_{m} A_{nm} \langle e_m|\psi\rangle . \qquad (\text{in the } \sum_j \text{ sum, only one } j = n \text{ term is nonzero}) \tag{B.39}$$

Hence, if we once again regard the components $\{\langle e_m|\psi\rangle\}$ as a column vector, the components of the output form another column vector produced by a product of the matrix A with the input column vector:

$$\begin{pmatrix} \langle e_1| \hat{A} |\psi\rangle \\ \vdots \\ \langle e_N| \hat{A} |\psi\rangle \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1N} \\ A_{21} & A_{22} & \dots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \dots & A_{NN} \end{pmatrix} \begin{pmatrix} \langle e_1|\psi\rangle \\ \vdots \\ \langle e_N|\psi\rangle \end{pmatrix}. \tag{B.40}$$

Some caveats about the ket-bra form:

(1) In rare cases in advanced quantum mechanics, we also need to deal with antilinear operators that are not linear and cannot be expressed in the ket-bra form, but we don't need them in this book.

(2) For infinite-dimensional Hilbert spaces, there exist operators that cannot be expressed in the ket-bra form exactly, such as the position operator of a particle. In physics, we deal with those using a trick by Dirac: define a continuous version of an orthonormal basis $\{|\boldsymbol{x}\rangle : \boldsymbol{x} \in \mathbb{R}^n\}$ that obeys

$$\langle \boldsymbol{x} | \boldsymbol{x}' \rangle = \delta^n(\boldsymbol{x} - \boldsymbol{x}'), \tag{B.41}$$

where δ^n is the n-dimensional Dirac delta function, and then express an operator as an integral rather then a sum:

$$\hat{A} = \iint A(\boldsymbol{x}, \boldsymbol{x}') |\boldsymbol{x}\rangle \langle \boldsymbol{x}'| \, d^n\boldsymbol{x} d^n\boldsymbol{x}', \tag{B.42}$$

where $A(\boldsymbol{x}, \boldsymbol{x}')$ is now a function of two variables $\boldsymbol{x}$ and $\boldsymbol{x}'$ rather than a matrix. Mathematicians hate this but it works.

There is a unique zero operator denoted by 0 (without the hat for brevity). It is defined by

$$0 |\psi\rangle = 0 \quad \forall |\psi\rangle \in \mathcal{H}. \tag{B.43}$$

In other words, when the zero operator is applied to any vector, the result is always the zero vector. It is slightly sloppy to use the same symbol 0 to denote the zero number, the zero vector, and the zero operator, but the notation is standard and harmless in practice; they all behave the same way as the number 0.

Be extremely careful that, like matrix algebra, you cannot interchange the order of two operators in a product usually:

$$\boxed{\hat{A}\hat{B} \neq \hat{B}\hat{A} \quad \text{usually.}} \tag{B.44}$$

In the rare cases that $\hat{A}\hat{B} = \hat{B}\hat{A}$, we say that the two operators **commute**. In general, noncommutativity is the single most annoying feature of quantum mechanics. Another way of describing this problem is to use the **commutator**, defined as

$$\boxed{[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.} \tag{B.45}$$

If $[\hat{A}, \hat{B}] = 0$ (the zero operator), then we say that $\hat{A}$ and $\hat{B}$ commute, and if the commutator is not zero, they don't commute.

Exercise B.8. Assume an orthonormal basis $\{|e_n\rangle : n = 1, \dots, N\}$ in the following.

(1) Show that the matrix representation of $\hat{A}$ is given by

$$\boxed{A_{nm} = \langle e_n | \hat{A} | e_m \rangle .} \tag{B.46}$$

In other words, there's a one-to-one correspondence between an operator $\hat{A}$ and its matrix representation A, as long as we fix an orthonormal basis.

(2) An identity operator $\hat{I}$ is defined by

$$\hat{I} |\psi\rangle = |\psi\rangle \tag{B.47}$$

for any $|\psi\rangle$. Prove that it can be expressed as

$$\boxed{\hat{I} = \sum_n |e_n\rangle \langle e_n| .} \tag{B.48}$$

Find the matrix representation of $\hat{I}$. Show that $\hat{I}$ commutes with any operator.

(3) Find the matrix representation of $\hat{A}\hat{B}$ in terms of the matrix representations of $\hat{A}$ and $\hat{B}$ if

$$\hat{A} = \sum_{n,m} A_{nm} |e_n\rangle \langle e_m| , \qquad \hat{B} = \sum_{n,m} B_{nm} |e_n\rangle \langle e_m| . \tag{B.49}$$

Exercise B.9. Let $\{|e_n\rangle : n = 1, \dots, N\}$ be a set of vectors in a Hilbert space that are not necessarily orthogonal or normalized. Suppose that the identity operator can be expressed as

$$\hat{I} = \sum_{n=1}^{N} |e_n\rangle \langle e_n| . \tag{B.50}$$

Then show that any vector $|\psi\rangle \in \mathcal{H}$ can be expressed as a linear combination of $\{|e_n\rangle\}$, i.e., $\{|e_n\rangle\}$ is a **complete** set of vectors of the Hilbert space, and Eq. (B.50) is called the completeness condition on a set of vectors.

Side note. *A complete and linearly independent set of vectors is called a basis of the vector space. Equivalently, a set of vectors $\{|e_n\rangle\}$ is a basis if and only if any $|\psi\rangle \in \mathcal{H}$ can be uniquely expressed as a linear combination of the set. In other words, we can write any vector as*

$$|\psi\rangle = \sum_{n=1}^{N} \psi_n |e_n\rangle , \tag{B.51}$$

and the coefficients $\{\psi_n\}$ are unique, such that no other linear combination of $\{|e_n\rangle\}$ gives the same $|\psi\rangle$. To check that a set of vectors is an orthonormal basis, we need to check that they are orthonormal and also they satisfy the completeness condition given by Eq. (B.50).

B.5. Adjoint

The adjoint of an operator, also called the Hermitian conjugate, is analogous to the conjugate transpose † of a matrix, and we use the same symbol †. To define it, it is easier to use mathematicians' notation of the inner product. Given an operator $\hat{A}$, its adjoint, denoted by $\hat{A}^\dagger$, is defined by the property

$$\left(\phi, \hat{A}\psi\right) = \left(\hat{A}^\dagger \phi, \psi\right) \quad \forall \psi, \phi \in \mathcal{H}. \tag{B.52}$$

To write this definition in the bra-ket notation, we first define the adjoint of the ket as the bra:

$$\boxed{\langle \phi| = |\phi\rangle^\dagger ,} \tag{B.53}$$

so that the inner product can be written as

$$\langle\phi|\psi\rangle = |\phi\rangle^\dagger |\psi\rangle . \tag{B.54}$$

Then $\hat{A}^\dagger$ is defined by the property

$$\boxed{\langle\phi| \hat{A} |\psi\rangle = \left(\hat{A}^\dagger |\phi\rangle\right)^\dagger |\psi\rangle \quad \forall |\psi\rangle , |\phi\rangle \in \mathcal{H}.} \tag{B.55}$$

The adjoint operator is useful because it gives us a new way to compute $\langle\phi| \hat{A} |\psi\rangle$:

(1) The usual way: Apply $\hat{A}$ to $|\psi\rangle$ first, and then compute the inner product between $|\phi\rangle$ and $\hat{A}|\psi\rangle$.
(2) The new way: Apply $\hat{A}^\dagger$ to $|\phi\rangle$ first, and then compute the inner product between $\hat{A}^\dagger|\phi\rangle$ and $|\psi\rangle$.

Here are some fundamental properties of the adjoint, similar to those of the conjugate transpose:

(1) Antilinearity: for any complex numbers c_1, c_2 and any operators $\hat{A}_1$ and $\hat{A}_2$,

$$\boxed{\left(c_1\hat{A}_1 + c_2\hat{A}_2\right)^\dagger = c_1^*\hat{A}_1^\dagger + c_2^*\hat{A}_2^\dagger.} \tag{B.56}$$

In other words, we can pull † inside a sum, but remember to take the complex conjugate of the coefficients.

(2) Involution († is its own inverse):

$$\boxed{\hat{A}^{\dagger\dagger} = \hat{A}.} \tag{B.57}$$

(3) Contravariance:

$$\boxed{(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger.} \tag{B.58}$$

You should go through Exercise B.10 to learn how to compute the adjoint in practice.

Exercise B.10. Let A be the matrix representation of $\hat{A}$ with respect to an orthonormal basis $\{|e_n\rangle\}$. Show that the matrix representation of $\hat{A}^\dagger$ is given by

$$\langle e_n| \hat{A}^\dagger |e_m\rangle = \left(\langle e_m| \hat{A} |e_n\rangle\right)^*, \tag{B.59}$$

so that we can write

$$\boxed{\hat{A}^\dagger = \sum_{n,m} \left(A^\dagger\right)_{nm} |e_n\rangle \langle e_m| ,} \tag{B.60}$$

where $A^\dagger$ is the **conjugate transpose** of the matrix A. In other words, the matrix of $\hat{A}^\dagger$ is the conjugate transpose of the matrix of $\hat{A}$.

Exercise B.11. An operator is said to be **Hermitian** if

$$\boxed{\hat{A} = \hat{A}^\dagger.} \tag{B.61}$$

Show that an operator is Hermitian if and only if its matrix representation is Hermitian.

Exercise B.12. The inverse of an operator is defined by $\hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I}$. Show that $\hat{A}^{-1}$ is the inverse of $\hat{A}$ if and only if their matrix representations are inverses of each other.

Exercise B.13. An operator is said to be **unitary** if

$$\boxed{\hat{U}^{-1} = \hat{U}^\dagger,} \tag{B.62}$$

such that

$$\boxed{\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I},} \tag{B.63}$$

where $\hat{I}$ is the identity operator. Show that an operator is unitary if and only if its matrix representation is unitary.

Exercise B.14. Let $\{|e_n\rangle\}$ be an orthonormal basis of a Hilbert space and $\hat{U}$ be a unitary operator. Define another set of operators as

$$\left|e'_n\right\rangle = \hat{U}\left|e_n\right\rangle, \quad n = 1, \ldots, N. \tag{B.64}$$

Show that $\{|e'_n\rangle\}$ is also an orthonormal basis. Conversely, given two orthonormal bases $\{|e_n\rangle\}$ $\{|e'_n\rangle\}$, show that there exists some unitary operator $\hat{U}$ such that the two bases are related by Eq. (B.64).

Exercise B.15. An operator $\hat{A}$ is said to be **normal** if

$$\boxed{\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}.} \tag{B.65}$$

In other words, a normal operator is defined by the property that it commutes with its adjoint. Show that an operator is normal if and only if its matrix representation is normal.

Exercise B.16. Show that any Hermitian operator is normal. Show that any unitary operator is normal.

Exercise B.17. Prove that, for any $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ and any operator $\hat{A}$,

$$\boxed{\left(\langle\phi|\,\hat{A}\,|\psi\rangle\right)^* = \langle\psi|\,\hat{A}^\dagger\,|\phi\rangle\,.} \tag{B.66}$$

Exercise B.18. Prove that

$$\left|\langle\phi|\,\hat{A}\,|\psi\rangle\right|^2 = \langle\psi|\,\hat{B}\,|\psi\rangle = \langle\phi|\,\hat{C}\,|\phi\rangle\,, \tag{B.67}$$

where

$$\hat{B} = \hat{A}^\dagger\,|\phi\rangle\,\langle\phi|\,\hat{A}, \qquad \hat{C} = \hat{A}\,|\psi\rangle\,\langle\psi|\,\hat{A}^\dagger. \tag{B.68}$$

Side note. *You should notice from the exercises that the Hermitian, unitary, and normal properties of an operator do not depend on the orthonormal basis you choose to express the operator. To put it another way, if an operator is Hermitian, its matrix representation is Hermitian regardless of which orthonormal basis you choose; same with unitarity, normality, etc. In mathematics, these intrinsic properties of an operator are usually defined using abstract algebra without looking at the matrix representation at all.*

B.6. Eigenvectors and eigenvalues

Given an operator $\hat{A}$, a ket $|\psi\rangle$ is said to be an eigenvector of $\hat{A}$ if

$$\boxed{\hat{A}\,|\psi\rangle = \lambda\,|\psi\rangle} \tag{B.69}$$

for some complex number λ. λ is then called the eigenvalue of $\hat{A}$ associated with the eigenvector $|\psi\rangle$. The most important example in quantum mechanics is, of course, the eigenvectors of the Hamiltonian operator and the eigenvalues. You should go through the following important exercise:

Exercise B.19. Let $\hat{A}$ be a normal operator. Show that there exists an orthonormal basis $\{|e_n\rangle\}$ such that $\hat{A}$ can be expressed in the **diagonal form**

$$\boxed{\hat{A} = \sum_n \lambda_n\,|e_n\rangle\,\langle e_n|\,,} \tag{B.70}$$

where each $|e_n\rangle$ is an eigenvector of $\hat{A}$ and λ_n is the eigenvalue of $\hat{A}$ associated with $|e_n\rangle$, i.e.,

$$\hat{A}\,|e_n\rangle = \lambda_n\,|e_n\rangle\,. \tag{B.71}$$

Note that Eq. (B.70) is now a single sum, not the double sum in the general ket-bra form. Show that the eigenvalues of $\hat{A}$ are the same as the eigenvalues of its matrix representation.

A function of a normal operator $f(\hat{A})$ is defined in terms of its diagonal form given by Eq. (B.70) as

$$\boxed{f(\hat{A}) = \sum_n f(\lambda_n) \left|e_n\right\rangle \left\langle e_n\right|.} \tag{B.72}$$

In other words, to compute $f(\hat{A})$, we express $\hat{A}$ in its diagonal form first, and then apply the function to each eigenvalue. The result is another operator. The most important example is probably the exponential:

$$\exp \hat{A} = \sum_n \exp(\lambda_n) \left|e_n\right\rangle \left\langle e_n\right|. \tag{B.73}$$

This is equivalent to the following:

$$\boxed{\exp \hat{A} = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}.} \tag{B.74}$$

which can be used as the general definition of the operator exponential valid for any operator, not just normal operators. The most important example in quantum mechanics is the unitary operator associated with the Hamiltonian

$$\hat{U} = \exp\left(-\frac{i}{\hbar}\hat{H}t\right). \tag{B.75}$$

Exercise B.20. Let $\hat{A}$ be a Hermitian operator. Show that all its eigenvalues are real.

Exercise B.21. Show that all the eigenvalues of $\hat{A}^\dagger \hat{A}$ are nonnegative.

Exercise B.22. Let $\hat{U}$ be a unitary operator. Show that all its eigenvalues have magnitude $|\lambda_n| = 1$.

Exercise B.23. Let $\hat{A}$ be a Hermitian operator. Show that $\exp\left(i\hat{A}\right)$ is unitary.

Exercise B.24. Find the matrix representation of $\exp \hat{A}$ in terms of the matrix representation of $\hat{A}$.

Exercise B.25. Let $\hat{U}$ be a unitary operator. Show that it can always be expressed as $\exp\left(i\hat{A}\right)$ with respect to some Hermitian operator $\hat{A}$.

Exercise B.26. Show that for any operator $\hat{A}$ and any unitary operator $\hat{U}$,

$$\boxed{\hat{U}(\exp \hat{A})\hat{U}^\dagger = \exp\left(\hat{U}\hat{A}\hat{U}^\dagger\right).} \tag{B.76}$$

Exercise B.27. If $\hat{A}$ is a Hermitian operator, $|\psi\rangle$ is an eigenvector of $\hat{A}$, and λ is the eigenvalue associated with it, show that $|\psi\rangle$ is also an eigenvector of $\exp\left(i\hat{A}\right)$. Show that the eigenvalue associated with $|\psi\rangle$ for the operator $\exp\left(i\hat{A}\right)$ is $\exp(i\lambda)$.

B.7. Miscellaneous concepts

(1) The **trace** of an operator is defined as

$$\operatorname{tr} \hat{A} = \sum_n \left\langle e_n\right| \hat{A} \left|e_n\right\rangle \tag{B.77}$$

given an orthonormal basis $\{|e_n\rangle\}$.

(2) A Hermitian operator with nonnegative eigenvalues is called a **positive-semidefinite** operator. If all the eigenvalues are strictly positive, we say that it is positive-definite.

The most important example of a positive-semidefinite operator is the density operator in quantum mechanics to describe the state of a quantum state that interacts with an environment (an open quantum system). The density operator is positive-semidefinite and has a trace equal to 1.

Exercise B.28. Show that the trace of an operator does not depend on the chosen basis, i.e., if there is another orthonormal bsis $\{|e'_n\rangle\}$ of the Hilbert space, the trace is also given by

$$\operatorname{tr} \hat{A} = \sum_n \langle e'_n| \hat{A} |e'_n\rangle . \tag{B.78}$$

If $\hat{A}$ is a normal operator with eigenvalues $\{\lambda_n\}$, prove that

$$\operatorname{tr} \hat{A} = \sum_n \lambda_n. \tag{B.79}$$

Exercise B.29. Find $\operatorname{tr} \hat{A}$ in terms of a matrix representation of $\hat{A}$.

Exercise B.30. Prove the linear property of trace: for any complex numbers c_1, c_2 and any operators $\hat{A}_1, \hat{A}_2$,

$$\operatorname{tr}(c_1\hat{A}_1 + c_2\hat{A}_2) = c_1(\operatorname{tr} \hat{A}_1) + (c_2 \operatorname{tr} \hat{A}_2). \tag{B.80}$$

Exercise B.31. Prove

$$\boxed{\operatorname{tr} (|\psi\rangle \langle\phi|) = \langle\phi|\psi\rangle .} \tag{B.81}$$

Exercise B.32. Prove the cyclic property of the trace: for any operators $\hat{A}, \hat{B}$,

$$\boxed{\operatorname{tr}(\hat{A}\hat{B}) = \operatorname{tr}(\hat{B}\hat{A}).} \tag{B.82}$$

Exercise B.33. Prove the unitary invariance of the trace: for any unitary operator $\hat{U}$ and any operator $\hat{A}$,

$$\operatorname{tr}(\hat{U}\hat{A}\hat{U}^\dagger) = \operatorname{tr}(\hat{A}). \tag{B.83}$$

Exercise B.34. Prove that an operator $\hat{A}$ is positive-semidefinite if and only if

$$\langle\psi| \hat{A} |\psi\rangle \geq 0 \quad \forall |\psi\rangle \in \mathcal{H}. \tag{B.84}$$

B.8. Tensor product

Suppose that we need to describe two **degrees of freedom** for a system, e.g., the spins of two electrons. For now, think of them as two classical random variables. Suppose that the first spin $s_A \in \{+1, -1\}$ has two possible values, and the second spin $s_B \in \{+1, -1\}$ also has two possible values. The set of all possible values (sample space) of the two spins (s_A, s_B) is the **Cartesian product** of the two sets

$$\{+1, -1\} \times \{+1, -1\} = \{(1, 1), (1, -1), (-1, 1), (-1, -1)\}. \tag{B.85}$$

In quantum mechanics, we generalize the concept of Cartesian product by the concept of **tensor product**. Suppose $\mathcal{H}_A$ and $\mathcal{H}_B$ are two Hilbert spaces that describe the sets of all possible states for two degrees of freedom. If $|\psi\rangle \in \mathcal{H}_A$ is the state of the first degree of freedom and $|\phi\rangle \in \mathcal{H}_B$ is the state of the second degree of freedom, then we can take the tensor product of the two vectors, denoted by

$$|\psi\rangle \otimes |\phi\rangle , \tag{B.86}$$

and say that this is a possible quantum state of the two degrees of freedom. It is also possible to do a superposition, i.e., a linear combination of states in the following way:

$$c_1 |a_1\rangle \otimes |b_1\rangle + c_2 |a_2\rangle \otimes |b_2\rangle , \quad c_1, c_2 \in \mathbb{C}. \tag{B.87}$$

In general, we say that $\mathcal{H}_A \otimes \mathcal{H}_B$ is the Hilbert space that contains the set of **all linear combinations of all the tensor products of two vectors, the first vector in $\mathcal{H}_A$ and the second vector in $\mathcal{H}_B$.**

To be more specific, suppose that $\{|e_n\rangle\}$ is an orthonormal basis of $\mathcal{H}_A$ and $\{|f_n\rangle\}$ is an orthonormal basis of $\mathcal{H}_B$. Then the tensor product of the two Hilbert spaces $\mathcal{H}_A \otimes \mathcal{H}_B$, which is also a Hilbert space, can be expressed as

$$\mathcal{H}_A \otimes \mathcal{H}_B = \left\{ \sum_{n,m} \psi_{nm} |e_n\rangle \otimes |f_m\rangle : \text{each } \psi_{nm} \in \mathbb{C} \right\}. \tag{B.88}$$

In other words,

$$\{|e_n\rangle \otimes |f_m\rangle : n = 1, \ldots, N, m = 1, \ldots, M\} \tag{B.89}$$

is an orthonormal basis of $\mathcal{H}_A \otimes \mathcal{H}_B$. Notice that there are now $N \times M$ vectors in the orthonormal basis. Notice also that there are far more vectors in the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$: any linear combination of the $N \times M$ vectors in the orthonormal basis is fair game. This is **an important property of the tensor product: $\mathcal{H}_A \otimes \mathcal{H}_B$ contains not only the tensor products of any two vectors in the two Hilbert spaces, but also all their linear combinations.**

Another fundamental property of the tensor product: Given any complex numbers $\{c_n\}$, $\{d_n\}$, and any sets of vectors $\{|a_n\rangle \in \mathcal{H}_A\}$ and $\{|b_n\rangle \in \mathcal{H}_B\}$, we can always write

$$\boxed{\left(\sum_n c_n |a_n\rangle\right) \otimes \left(\sum_m d_m |b_m\rangle\right) = \sum_{n,m} c_n d_m |a_n\rangle \otimes |b_m\rangle .} \tag{B.90}$$

In other words, we can always **convert the tensor product of two sums into a double sum**.

The third important property of the tensor product has to do with how we take the inner product. Let $|a_1\rangle, |a_2\rangle \in \mathcal{H}_A$ and $|b_2\rangle, |b_2\rangle \in \mathcal{H}_B$. Take the tensor product of $|a_1\rangle \in \mathcal{H}_A$ with $|b_1\rangle \in \mathcal{H}_B$ to get $|a_1\rangle \otimes |b_1\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, and take the tensor product of $|a_2\rangle \in \mathcal{H}_A$ with $|b_2\rangle \in \mathcal{H}_B$ to get $|a_2\rangle \otimes |b_2\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. The inner product is given by

$$\boxed{(\langle a_1| \otimes \langle b_1|)(|a_2\rangle \otimes |b_2\rangle) = \langle a_1|a_2\rangle \langle b_1|b_2\rangle .} \tag{B.91}$$

In other words, **we take the inner product $\langle a_1|a_2\rangle$ and $\langle b_1|b_2\rangle$ in each Hilbert subspace first to obtain two complex numbers, and then take the product of the two complex numbers.**

To make the notations look nicer, I will write each vector in the orthonormal basis as

$$|e_n, f_m\rangle \equiv |e_n\rangle \otimes |f_m\rangle . \tag{B.92}$$

The bra can be written as

$$\langle e_n, f_m| = |e_n, f_m\rangle^\dagger = \langle e_n| \otimes \langle f_m| , \tag{B.93}$$

and the orthonormality of these vectors can be expressed as

$$\langle e_n, f_m|e_{n'}, f_{m'}\rangle = \delta_{nn'}\delta_{mm'}. \tag{B.94}$$

If $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ describes the quantum state of two degrees of freedom, then we can always write

$$|\psi\rangle = \sum_{n,m} \psi_{nm} |e_n, f_m\rangle . \tag{B.95}$$

in terms of the orthonormal basis $\{|e_n, f_m\rangle\}$ and the components ψ_{nm}, which are given by

$$\psi_{nm} = \langle e_n, f_m|\psi\rangle . \tag{B.96}$$

Then we say that ψ_{nm} is the wavefunction of the two degrees of freedom n and m.

In general, if we write two vectors in $\mathcal{H}_A \otimes \mathcal{H}_B$ as

$$|\psi\rangle = \sum_{n,m} \psi_{nm} |e_n, f_m\rangle , \tag{B.97}$$

$$|\phi\rangle = \sum_{n,m} \phi_{nm} |e_n, f_m\rangle , \tag{B.98}$$

Then you should be able to show that their inner product is

$$\boxed{\langle\phi|\psi\rangle = \sum_{n,m} \phi^*_{nm}\psi_{nm}.} \tag{B.99}$$

With the orthonormal basis, we can also write any operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ in the ket-bra form:

$$\hat{A} = \sum_{n,m,n',m'} A_{nmn'm'} |e_n, f_m\rangle \langle e_{n'}, f_{m'}| . \tag{B.100}$$

The matrix representation now has four indices. If we take a tensor product of multiple Hilbert spaces, the number of indices will explode! You should begin to see why we prefer to use the abstract bra-ket notation—we don't want to write all the indices everytime we specify an operator, and the notations of matrix algebra are becoming inadequate to fully handle what's going on.

Another way of making up an operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ is to take an operator $\hat{A}$ on $\mathcal{H}_A$ and another operator $\hat{B}$ on $\mathcal{H}_B$ and then form the tensor product $\hat{A} \otimes \hat{B}$, which is an operator on $\mathcal{H}_A \otimes \mathcal{H}_B$. It has this fundamental property:

$$\boxed{(\hat{A} \otimes \hat{B}) |\psi\rangle \otimes |\phi\rangle = (\hat{A} |\psi\rangle) \otimes (\hat{B} |\phi\rangle).} \tag{B.101}$$

In other words, as long as both $\hat{A} \otimes \hat{B}$ and $|\psi\rangle \otimes |\phi\rangle$ are tensor products, we can apply $\hat{A}$ to $|\psi\rangle$ and $\hat{B}$ to $|\phi\rangle$ separately and then put them back together. All the other properties of $\hat{A} \otimes \hat{B}$ can be derived from this. A common example is $\hat{A} \otimes \hat{I}$, where $\hat{I}$ is the identity operator on $\mathcal{H}_B$. It applies $\hat{A}$ to the $\mathcal{H}_A$ part and leaves the $\mathcal{H}_B$ part alone.

Some handy identities are as follows:

$$\boxed{\left(\sum_n c_n \hat{A}_n\right) \otimes \left(\sum_m d_m \hat{B}_m\right) = \sum_{n,m} c_n d_m \hat{A}_n \otimes \hat{B}_m.} \tag{B.102}$$

$$\boxed{(\hat{A} \otimes \hat{B})(\hat{C} \otimes \hat{D}) = (\hat{A}\hat{C}) \otimes (\hat{B}\hat{D}).} \tag{B.103}$$

$$\boxed{(|a_1\rangle \otimes |b_1\rangle)(\langle a_2| \otimes \langle b_2|) = (|a_1\rangle \langle a_2|) \otimes (|b_1\rangle \langle b_2|).} \tag{B.104}$$

When we have an operator $\hat{A}$ on $\mathcal{H}_A$, we often abbreviate $\hat{A} \otimes \hat{I}$ on the big Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ as just $\hat{A}$. Similarly, when we have an operator $\hat{A}$ on $\mathcal{H}_A$ and an operator $\hat{B}$ on $\mathcal{H}_B$, we often abbreviate $\hat{A} \otimes \hat{B}$ as $\hat{A}\hat{B}$. What we really mean by $\hat{A}\hat{B}$ in that context is then

$$\boxed{\hat{A}\hat{B} = (\hat{A} \otimes \hat{I})(\hat{I} \otimes \hat{B}) = \hat{A} \otimes \hat{B}.} \tag{B.105}$$

It's a bit ambiguous but such abbreviation is standard; otherwise we'd have to write really long formulas with tons of $\otimes$ and $\hat{I}$.

The math may be a bit dry and tedious, but keep this general meaning in mind: we use the tensor product to combine multiple degrees of freedom together. The tensor product is in fact how we define degrees of freedom in quantum mechanics: if a Hilbert space can be decomposed as a tensor product $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \ldots$, then each constituent $\mathcal{H}_j$ corresponds to a degree of freedom. For example, a 3D particle has a state in the Hilbert space $\mathcal{H}_x \otimes \mathcal{H}_y \otimes \mathcal{H}_z$ that can be expressed as $\iiint \psi(x,y,z) |x\rangle \otimes |y\rangle \otimes |z\rangle \, d^3\boldsymbol{r}$, so the three Hilbert spaces represent three degrees of freedom; we don't count the momenta separately. If the particle has spin, we attach another Hilbert space for the spin via the tensor product.

Exercise B.35. Prove

$$\operatorname{tr}(\hat{A} \otimes \hat{B}) = (\operatorname{tr} \hat{A})(\operatorname{tr} \hat{B}). \tag{B.106}$$

Exercise B.36. Given $\hat{A} = \hat{B} \otimes \hat{C}$, write the matrix representation A of $\hat{A}$ in Eq. (B.100) in terms of the matrix representations of $\hat{B}$ and $\hat{C}$, if

$$\hat{B} = \sum_{n,n'} B_{nn'} |e_n\rangle \langle e_{n'}|, \qquad \hat{C} = \sum_{m,m'} C_{mm'} |e_m\rangle \langle e_{m'}|. \tag{B.107}$$

B.9. Isomorphism

Consider two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. An operator $\hat{U} : \mathcal{H}_A \to \mathcal{H}_B$ is said to be unitary if $\hat{U}^\dagger \hat{U} = \hat{I}_A$ and $\hat{U}\hat{U}^\dagger = \hat{I}_B$, where $\hat{I}_x$ with any subscript x is the identity operator on $\mathcal{H}_x$. $\hat{U}$ is a bijective operator and also preserves the inner product, since

$$\langle\phi| \hat{U}^\dagger \hat{U} |\psi\rangle = \langle\phi|\psi\rangle. \tag{B.108}$$

For example, for real Euclidean vectors in $\mathbb{R}^n$, the dot product is an inner product, and the preservation of the inner product means that the length of a vector is preserved through the unitary operator, and also the angle between any two vectors is preserved. A unitary operator in that case is represented by an orthogonal matrix, which models any rotation, permutation of components, and sign flip of each component.

Two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ are said to be isomorphic, denoted as $\mathcal{H}_A \sim \mathcal{H}_B$ or more sloppily $\mathcal{H}_A = \mathcal{H}_B$, if a unitary operator $\hat{U} : \mathcal{H}_A \to \mathcal{H}_B$ exists. Then there is a bijective relation $\hat{U}$ between the two spaces and the bijection preserves the inner product.

Two isomorphic Hilbert spaces are effectively the same; we consider isomorphic spaces because one may be more natural or convenient to use than the other, much like the use of an orthogonal matrix to transform the Cartesian coordinates.

Exercise B.37. Prove that $\mathbb{C}^n$ with inner product

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle \equiv \sum_{j=1}^{n} u_j^* v_j \tag{B.109}$$

is isomorphic to any complex Hilbert space $\mathcal{H}$ with n dimensions.

Exercise B.38. Prove

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \sim \mathcal{H}_2 \otimes \mathcal{H}_1. \tag{B.110}$$

B.10. Partial operations

B.10.1. Partial ket and bra. Consider a tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$ of Hilbert spaces. Let $|b\rangle \in \mathcal{H}_B$. Given $|b\rangle$, the **partial ket** $|b\rangle : \mathcal{H}_A \to \mathcal{H}_A \otimes \mathcal{H}_B$ is an operator defined by

$$\boxed{|b\rangle\,|a\rangle \equiv |a\rangle \otimes |b\rangle\,, \quad \forall\, |a\rangle \in \mathcal{H}_A.} \tag{B.111}$$

In other words, the partial ket just appends $|b\rangle$ via a tensor product. This partial-ket operator is simply written as $|b\rangle$; it's slightly sloppy but it works as far as I know. The **partial bra** $\langle b| : \mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{H}_A$ is then defined as the adjoint of the partial ket, and it turns out to be given by

$$\boxed{\langle b|\,(|a\rangle \otimes |c\rangle) \equiv (\langle b|c\rangle)\,|a\rangle\,,} \quad \forall\, |a\rangle \in \mathcal{H}_A, |c\rangle \in \mathcal{H}_B. \tag{B.112}$$

In other words, given any tensor product $|a\rangle \otimes |c\rangle$, the partial bra takes the inner product of $|b\rangle$ with $|c\rangle$ and leaves $|a\rangle$ alone.

B.10.2. Partial trace. Given an operator $\hat{A} : \mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{H}_A \otimes \mathcal{H}_B$ on a tensor-product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, the partial trace of $\hat{A}$ with respect to $\mathcal{H}_B$ produces an operator on $\mathcal{H}_A$ and is defined by the fundamental property

$$\boxed{\mathrm{tr}\left[\hat{A}(\hat{O} \otimes \hat{I})\right] = \mathrm{tr}\left[\left(\mathrm{tr}_B\,\hat{A}\right)\hat{O}\right],} \tag{B.113}$$

where $\hat{O}$ is any operator on $\mathcal{H}_A$ and $\hat{I}$ is the identity operator on $\mathcal{H}_B$. In quantum mechanics, it is mainly used on a density operator, such that

$$\boxed{\mathrm{tr}\left[\hat{\rho}(\hat{O} \otimes \hat{I})\right] = \mathrm{tr}\left[(\mathrm{tr}_B\,\hat{\rho})\hat{O}\right].} \tag{B.114}$$

This expression means that, if $\hat{\rho}$ is the state of two degrees of freedom and we want to compute the expected value of $\hat{O}$ for the first degree of freedom, then we can "trace out" the second degree of freedom by computing $\mathrm{tr}_B\,\hat{\rho}$ first. The partial trace is one of the most important operations in open quantum system theory.

Given an orthonormal basis $\{|f_m\rangle\}$ in $\mathcal{H}_B$, a recipe for the partial trace is

$$\boxed{\mathrm{tr}_B\,\hat{A} = \sum_l \langle f_l|\,\hat{A}\,|f_l\rangle\,,} \tag{B.115}$$

where $\langle f_l|$ and $|f_l\rangle$ are partial bra and ket operators. With $\hat{A}$ in the ket-bra form given by Eq. (B.100), the partial trace becomes

$$\operatorname{tr}_B \hat{A} = \sum_l \langle f_l| \left(\sum_{n,m,n',m'} A_{nmn'm'} |e_n, f_m\rangle \langle e_{n'}, f_{m'}| \right) |f_l\rangle \tag{B.116}$$

$$= \sum_l \sum_{n,m,n',m'} A_{nmn'm'} \langle f_l| (|e_n\rangle \otimes |f_m\rangle)(\langle e_{n'}| \otimes \langle f_{m'}|) |f_l\rangle \tag{B.117}$$

$$= \sum_l \sum_{n,n'} A_{nln'l} |e_n\rangle \langle e_{n'}| . \tag{B.118}$$

If an operator is a tensor product $\hat{A} \otimes \hat{B}$, the partial trace is especially simple:

$$\boxed{\operatorname{tr}_B(\hat{A} \otimes \hat{B}) = (\operatorname{tr} \hat{B})\hat{A}.} \tag{B.119}$$

This is handy if the density operator is given by $\rho = \hat{\rho}_A \otimes \hat{\rho}_B$ with $\operatorname{tr} \hat{\rho}_A = 1$ and $\operatorname{tr} \hat{\rho}_B = 1$,

$$\operatorname{tr}_B(\hat{\rho}_A \otimes \hat{\rho}_B) = (\operatorname{tr} \hat{\rho}_B)\hat{\rho}_A = \hat{\rho}_A. \tag{B.120}$$

We say that the state is a product state if the density operator is a tensor product. We use it to model **independent** degrees of freedom, since the expected value of any $\hat{O}$ for one degree of freedom becomes

$$\operatorname{tr}\left[(\hat{O} \otimes \hat{I})(\hat{\rho}_A \otimes \hat{\rho}_B)\right] = \operatorname{tr}\left(\hat{O}\hat{\rho}_A\right), \tag{B.121}$$

which does not depend on $\hat{\rho}_B$ at all.

Exercise B.39. Prove that the partial trace also has a cyclic property in the form

$$\operatorname{tr}_B\left[\left(\hat{I} \otimes \hat{B}\right)\hat{O}\right] = \operatorname{tr}_B\left[\hat{O}\left(\hat{I} \otimes \hat{B}\right)\right], \tag{B.122}$$

if $\hat{O}$ is an operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ and $\hat{B}$ is an operator on $\mathcal{H}_B$.

(Beware that, for a partial trace, the operator being cycled needs to be in the form of $\hat{I} \otimes \hat{B}$.)

Exercise B.40. Prove

$$\hat{A}_1\left(\operatorname{tr}_B \hat{O}\right)\hat{A}_2 = \operatorname{tr}_B\left[\left(\hat{A}_1 \otimes \hat{I}\right)\hat{O}\left(\hat{A}_2 \otimes \hat{I}\right)\right], \tag{B.123}$$

where $\hat{O}$ is on $\mathcal{H}_A \otimes \mathcal{H}_B$ while $\hat{A}_1$ and $\hat{A}_2$ are on $\mathcal{H}_A$.

B.11. Direct sum

Another way of combining two vectors $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$ in two different Hilbert spaces is the direct sum

$$|a\rangle \oplus |b\rangle . \tag{B.124}$$

It is defined by the property that, given $|a_1\rangle, |a_2\rangle \in \mathcal{H}_A$ and $|b_1\rangle, |b_2\rangle \in \mathcal{H}_B$,

$$(\langle a_1| \oplus \langle b_1|)(|a_2\rangle \oplus |b_2\rangle) = \langle a_1|a_2\rangle + \langle b_1|b_2\rangle , \tag{B.125}$$

This is similar to Eq. (B.91) for the tensor product, except that we sum the two inner products here. The set of all such direct sums is also a Hilbert space and denoted as

$$\mathcal{H}_A \oplus \mathcal{H}_B \equiv \{|a\rangle \oplus |b\rangle : |a\rangle \in \mathcal{H}_A, |b\rangle \in \mathcal{H}_B\}. \tag{B.126}$$

We don't use the direct sum as much as the tensor product in quantum mechanics, but it is quite useful in linear algebra and probability theory. In those areas, we usually consider two special cases:

(1) The direct sum of two column vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, which is simply the concatenation

$$\boxed{\boldsymbol{a} \oplus \boldsymbol{b} \equiv \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix}.} \tag{B.127}$$

(2) The direct sum of two square matrices A and B, defined as

$$\boxed{A \oplus B \equiv \begin{pmatrix} A & \\ & B \end{pmatrix},} \tag{B.128}$$

where the rest of the entries are zero.

These definitions agree with the abstract definition if we assume the inner product $\langle \boldsymbol{y}, \boldsymbol{x} \rangle \equiv \boldsymbol{y}^\dagger \boldsymbol{x}$ for column vectors and $\langle Y, X \rangle \equiv \operatorname{tr}(Y^\dagger X)$ for square matrices, where $\dagger$ is the conjugate transpose.

One application of the direct sum is in probability theory: if we have two column vector of random variables $\boldsymbol{X}$ and $\boldsymbol{Y}$, we can use the direct sum $\boldsymbol{X} \oplus \boldsymbol{Y}$ to form one big column vector of all the random variables. If the covariance matrix of $\boldsymbol{X}$ is $\Sigma^{(X)}$, the covariance matrix of $\boldsymbol{Y}$ is $\Sigma^{(Y)}$, and there is no covariance between any entry of $\boldsymbol{X}$ and any entry of $\boldsymbol{Y}$, then the covariance matrix of $\boldsymbol{X} \oplus \boldsymbol{Y}$ is $\Sigma^{(X)} \oplus \Sigma^{(Y)}$.

Exercise B.41. Let $\boldsymbol{a}$ be a column vector with n entries, $\boldsymbol{b}$ be a column vector with m entries, A, A' be $n \times n$ matrices, and B, B' be $m \times m$ matrices. Show that

(1)

$$(A \oplus B)(\boldsymbol{a} \oplus \boldsymbol{b}) = (A\boldsymbol{a}) \oplus (B\boldsymbol{b}). \tag{B.129}$$

(2)

$$(A \oplus B)(A' \oplus B') = (AA') \oplus (BB'). \tag{B.130}$$

(3)

$$(A \oplus B)^{-1} = (A^{-1}) \oplus (B^{-1}). \tag{B.131}$$

B.12. Positive-semidefinite operators*

An important class of operators in open quantum systems theory are called positive-semidefinite operators. The most important example is the density operator, which models the state of an open quantum system.

For a complex Hilbert space $\mathcal{H}$, an operator is said to be positive-semidefinite if

$$\hat{A} = \hat{A}^\dagger \quad \text{and} \quad \langle \psi | \hat{A} | \psi \rangle \geq 0 \quad \forall |\psi\rangle \in \mathcal{H}. \tag{B.132}$$

The first equality means that $\hat{A}$ is self-adjoint, so that $\langle \psi | \hat{A} | \psi \rangle$ is real for any $|\psi\rangle \in \mathcal{H}$. If it is not self-adjoint, $\langle \psi | \hat{A} | \psi \rangle$ may be complex, and the inequality would not make sense. Any self-adjoint $\hat{A}$ has the eigenvalue decomposition

$$\hat{A} = \sum_n \lambda_n |e_n\rangle \langle e_n| . \tag{B.133}$$

Then $\hat{A}$ is positive-semidefinite if and only if all eigenvalues of $\hat{A}$ are nonnegative, i.e., $\lambda_n \geq 0$ for all n. A shorthand for positive-semidefiniteness is

$$\hat{A} \geq 0. \tag{B.134}$$

Similarly, we define a positive-definite operator by

$$\hat{A} = \hat{A}^\dagger \quad \text{and} \quad \langle \psi | \hat{A} | \psi \rangle > 0 \quad \forall |\psi\rangle \in \mathcal{H} : |\psi\rangle \neq 0. \tag{B.135}$$

A self-adjoint operator is positive-definite if and only if all its eigenvalues are strictly positive. As a shorthand, we write

$$\hat{A} > 0. \tag{B.136}$$

For two positive-semidefinite operators $\hat{A}, \hat{B}$, the inequality

$$\hat{A} \geq \hat{B} \tag{B.137}$$

means that $\hat{A} - \hat{B}$ is positive-semidefinite; $\hat{A} > \hat{B}$ means that $\hat{A} - \hat{B}$ is positive-definite. The notation is justified because such a relation is indeed a partial order (https://en.wikipedia.org/wiki/Partially_ordered_set).

B.13. Positive-semidefinite matrices*

Complex positive-semidefinite matrices are defined in the same way if we take $\mathcal{H} = \mathbb{C}^n$ to be the space of complex column vectors and the inner product to be

$$\langle \boldsymbol{\phi}, \boldsymbol{\psi} \rangle = \boldsymbol{\phi}^\dagger \boldsymbol{\psi}. \tag{B.138}$$

In other words, a matrix A is said to be positive-semidefinite if

$$A = A^\dagger, \qquad\qquad \boldsymbol{\psi}^\dagger A \boldsymbol{\psi} \geq 0 \quad \forall \boldsymbol{\psi} \in \mathbb{C}^n, \tag{B.139}$$

and we write $A \geq 0$. A self-adjoint matrix is positive-semidefinite if and only if all its eigenvalues are all nonnegative.

All the above statements remain valid for a positive-definite matrix if we replace $\geq$ by $>$ and assume $\boldsymbol{\psi} \neq 0$.

If the Hilbert space is real, things get tricker. Since we will deal with real Hilbert spaces only in the context of matrix algebra, let's assume that $\mathcal{H} = \mathbb{R}^n$ is the Hilbert space of real column vectors, and the inner product is defined as

$$\langle \boldsymbol{\phi}, \boldsymbol{\psi} \rangle = \boldsymbol{\phi}^\top \boldsymbol{\psi}. \tag{B.140}$$

A real matrix is said to be positive-semidefinite with respect to the real Hilbert space if

$$\boldsymbol{\psi}^\top A \boldsymbol{\psi} \geq 0 \quad \forall \boldsymbol{\psi} \in \mathbb{R}^n. \tag{B.141}$$

The definition no longer requires A to be self-adjoint or symmetric ($A = A^\top$). An example in physics is the Onsager transport matrix (https://en.wikipedia.org/wiki/Onsager_reciprocal_relations), which is always positive-semidefinite but may not be symmetric.

The covariance matrix of real random variables is an important example that is both positive-semidefinite and symmetric.

In all cases, we can still write

$$A \geq B \tag{B.142}$$

if $A - B$ is positive-semidefinite, or write $A > B$ if $A - B$ is positive-definite.

B.14. Message to mathematicians

If you are a mathematician or going into mathematical physics, you should be cautioned that I have presented a lot of the concepts backwards and with little rigor or generality, relying a lot on orthonormal bases and matrix representations.

For finite-dimensional Hilbert spaces ($N < \infty$), the abstract formalism is isomorphic to matrix algebra, so my approach is quite safe. When the Hilbert spaces are **infinite-dimensional**, however, mathematicians worry a lot more about when and how infinite sums may converge. If that is the way you like your math, please consult textbooks written by mathematicians instead, such as Refs. [39, 40].

APPENDIX C

Probability

C.1. Axioms

The set of all possible outcomes of an experiment, commonly denoted as Ω, is called the **sample space**, e.g., $\Omega = \{1, 2, 3, 4, 5, 6\}$ for a dice throw.

An event is a set of outcomes and a subset of Ω, e.g., an even-number event for a dice throw is the set $\{2, 4, 6\}$. The set of all events is called the **event space** F. It also has the fancy name σ-algebra in mathematics.

When both A AND B occur, we model the event as the intersection of the two sets, i.e.,

$$(A \text{ and } B) = (A \cap B). \tag{C.1}$$

When A OR B occurs, we model the event as the union of the two sets, i.e.,

$$(A \text{ or } B) = (A \cup B). \tag{C.2}$$

F is assumed to include any set that results from such operations on its elements.

If the sample space contains a countable number of outcomes, we usually assume that the event space F is the power set of Ω, i.e., the set of all subsets of Ω. For example, for a coin flip,

$$\Omega = \{\text{head}, \text{tail}\}, \qquad F = \{\varnothing, \{\text{head}\}, \{\text{tail}\}, \Omega\}, \tag{C.3}$$

and for a sample space with 3 elements,

$$\Omega = \{1, 2, 3\}, \qquad F = \{\varnothing, 1, 2, 3, \{1, 2\}, \{2, 3\}, \{1, 3\}, \Omega\}. \tag{C.4}$$

If Ω contains an uncountable number of outcomes, e.g., when $\Omega = \mathbb{R}$, then a rigorous definition of F is a lot more complicated for mathematical reasons. Fortunately, such a rigorous definition of F is seldom important or necessary in physics; we can just assume that F contains all the subsets of Ω that we need in reality.

The probability $P[A]$ is a function that assigns a number to each event $A \in F$. The **Kolmogorov axioms** for probability are as follows:

(1) The probability of any event is nonnegative.
(2) The probability of anything happening is 1, i.e., $P[\Omega] = 1$.
(3) Given two mutually exclusive events ($A \cap B = \varnothing$),

$$P[A \cup B] = P[A] + P[B]. \tag{C.5}$$

Everything in probability theory can be derived from the three axioms, at least in principle.

It is useful to picture $P[A]$ as the amount of stuff in an area, e.g., sand on a beach. Let Ω be the whole beach and $A \subseteq \Omega$ be a subarea of the beach. Then

(1) Axiom (1) says that the amount of sand on any area is always nonnegative.
(2) Axiom (2) says that the total amount $P[\Omega]$ on the whole beach is normalized as 100% (such that the amount on any area is always expressed as a fraction of the total amount).
(3) Axiom (3) says that, if two areas are disjoint (i.e., no overlap), we can count the total amount of sand $P[A \cup B]$ on the two areas by counting the amount on each area ($P[A]$ and $P[B]$) and then summing the two amounts.

Since we often deal with the three objects (Ω, F, P) together, we call (Ω, F, P) a **probability space**.

C.2. Random variables

Any function $X : \Omega \to \mathbb{R}^n$ that maps an outcome to a vector of numbers is called a random variable. For simplicity, we assume in this chapter that Ω itself is a set of numbers, e.g., $\Omega = \mathbb{R}^n$, so that the outcome is a random variable.

We usually use a capital letter such as X to denote a random variable, although we will be a bit sloppier in other chapters.

If Ω is countable, e.g., $\Omega = \mathbb{N}_0 = \{0, 1, 2, \dots\}$, then we say that the random variable is a **discrete variable**. We can define a **probability mass function** $P_X(x)$ as the probability that X is equal to a specific value $x \in \Omega$:

$$\boxed{P_X(x) = P[X = x].} \tag{C.6}$$

The probability of an event is then the sum of all the probabilities of outcomes in the event:

$$\boxed{P[X \in A] = \sum_{x \in A} P_X(x).} \tag{C.7}$$

To compute the **expected value** of a random variable, we do

$$\boxed{\mathbb{E}(X) = \sum_{x \in \Omega} x P_X(x).} \tag{C.8}$$

More generally, a function $g(X)$ of the random variable is another random variable, and its expected value is given by

$$\boxed{\mathbb{E}[g(X)] = \sum_{x \in \Omega} g(x) P_X(x).} \tag{C.9}$$

If $\Omega = \mathbb{R}^n$, we say that X is a **continuous variable**, and we use a **probability density** $f_X(\boldsymbol{x})$ instead. Think of $f_X(\boldsymbol{x})d^n\boldsymbol{x}$ as the probability that X is in a tiny n-dimensional cube around $\boldsymbol{x}$, and $d^n\boldsymbol{x}$ is the volume of the cube. We can convert any formula in terms of P_X to the corresponding formula in terms of f_X using the following rules:

(1) Replace $P_X(x)$ by $f_X(\boldsymbol{x})d^n\boldsymbol{x}$.
(2) Replace $\sum_{x \in A}$ by $\int_A$.

The probability that X is in a region $A \subseteq \mathbb{R}^n$ can then be expressed as the integral

$$\boxed{P[X \in A] = \int_A f_X(\boldsymbol{x}) d^n\boldsymbol{x},} \tag{C.10}$$

and the expected value of any function of X can be expressed as

$$\boxed{\mathbb{E}[g(X)] = \int g(\boldsymbol{x}) f_X(\boldsymbol{x}) d^n\boldsymbol{x}.} \tag{C.11}$$

Regardless of the type of the random variable, the algebra of the expectation can be summarized in three rules:

(1) The expected value of a constant is the constant itself, i.e.,

$$\boxed{\mathbb{E}(a) = a,} \tag{C.12}$$

because a constant can be considered as a special case of a random variable whose outcome is deterministic, i.e., it always gives the same value.

(2) Given any two random variables X and Y,

$$\boxed{\mathbb{E}(X + Y) = \mathbb{E}(X) + \mathbb{E}(Y).} \tag{C.13}$$

Note that this formula works regardless of whether they are independent.

(3) We can pull any constant out of the expectation:

$$\boxed{\mathbb{E}(aX) = a\,\mathbb{E}(X).} \tag{C.14}$$

The latter two rules mean that the expectation $\mathbb{E}$ is a **linear** operation. Note that the result of an expectation is a constant, i.e., it's no longer random, so we have

$$\mathbb{E}[\mathbb{E}(X)] = \mathbb{E}(X). \tag{C.15}$$

A common measure of the randomness of a random variable is the **variance**, which is defined as

$$\boxed{\mathbb{V}(X) \equiv \mathbb{E}\left\{[X - \mathbb{E}(X)]^2\right\} = \mathbb{E}(X^2) - [\mathbb{E}(X)]^2.} \tag{C.16}$$

C.3. Multiple random variables

Consider two random variables X and Y. Let the sample and event spaces for X be (Ω_X, F_X), and those for Y be (Ω_Y, F_Y). The joint sample space for (X, Y) is the **Cartesian product**

$$\Omega = \Omega_X \times \Omega_Y \equiv \{(x, y) : x \in \Omega_X, y \in \Omega_Y\}. \tag{C.17}$$

The joint event space F is a set of subsets of Ω; we commonly write the joint event space as the tensor product

$$F = F_X \otimes F_Y. \tag{C.18}$$

For example, if $\Omega_X = \Omega_Y = \mathbb{R}$, then $\Omega = \Omega_X \times \Omega_y = \mathbb{R}^2$ is the two-dimensional plane, and any $C \in F$ is a two-dimensional area on the plane. In particular, the joint event $(X \in A) \cap (Y \in B)$ is modeled as

$$[(X \in A) \cap (Y \in B)] = [(X, Y) \in A \times B], \tag{C.19}$$

where $A \times B$ is the Cartesian product of $A \in F_X$ and $B \in F_Y$. Such a Cartesian product of events is called a rectangle event, because it looks like a rectangle when $\Omega_X = \Omega_Y = \mathbb{R}$ and A and B are intervals, as illustrated in Fig. C.1.

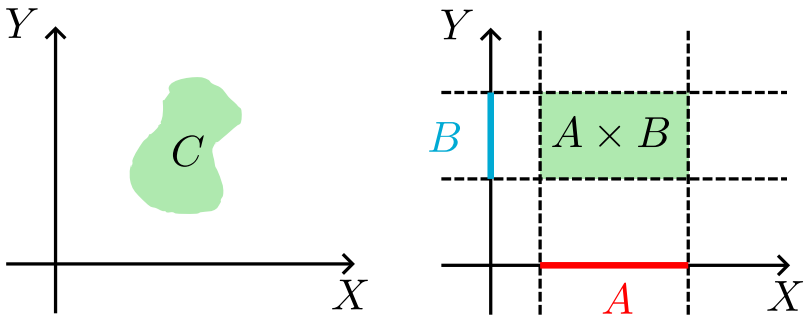

FIGURE C.1. For a joint sample space $\Omega_X \times \Omega_Y = \mathbb{R}^2$, an event $C \in F = F_X \otimes F_Y$ is an arbitrary area on the two-dimensional plane (left). A rectangle event $A \times B$ for intervals $A \in F_X$ and $B \in F_Y$ is the rectangle $\{(x, y) : x \in A \text{ and } y \in B\}$ (right).

Let the joint probability measure for (X, Y) on $(\Omega_X \times \Omega_Y, F_X \otimes F_Y)$ be P_{XY}, defined as

$$P_{XY}[C] \equiv P[(X, Y) \in C], \quad C \in F_X \otimes F_Y. \tag{C.20}$$

Then the probability of each rectangle event is

$$P[(X \in A) \cap (Y \in B)] = P_{XY}[A \times B]. \tag{C.21}$$

The marginal probability measures for X and Y become

$$P_X[A] \equiv P_{XY}[A \times \Omega_Y], \quad A \in F_X, \qquad\qquad P_Y[B] \equiv P_{XY}[\Omega_X \times B], \quad B \in F_Y, \tag{C.22}$$

respectively. If P_{XY} is separable for all rectangle events in the sense of

$$P_{XY}[A \times B] = P_X[A]P_Y[B] \quad \forall A \in F_X, B \in F_Y, \tag{C.23}$$

then we say that X and Y are **independent**.

Conversely, given a probability space (Ω_X, F_X, P_X) for X and a probability space (Ω_Y, F_Y, P_Y) for Y, we can form a **product measure** P_{XY} on $(\Omega_X \times \Omega_Y, F_X \otimes F_Y)$ so that it obeys Eq. (C.23) for all rectangle events, meaning that X and Y are assumed to be independent. Eq. (C.23) is sufficient to specify the probability measure for all rectangle or non-rectangle events, since we can divide up any $C \in F_X \otimes F_Y$ into tiny rectangle events and sum up the probabilities P_{XY} on them. We commonly write such a product measure as the tensor product

$$P_{XY} = P_X \otimes P_Y. \tag{C.24}$$

C.3.1. Discrete variables. The easiest case is when both X and Y are discrete. Then we can simply consider the joint probability mass function

$$\boxed{P_{XY}(x, y) \equiv P[(X = x) \cap (Y = y)],} \tag{C.25}$$

which gives

$$P[(X, Y) \in C] = \sum_{(x,y)\in C} P_{XY}(x, y), \qquad P_X(x) = \sum_y P_{XY}(x, y), \qquad P_Y(y) = \sum_x P_{XY}(x, y). \tag{C.26}$$

(X, Y) are independent if and only if the joint distribution is separable in the sense of

$$P_{XY}(x, y) = P_X(x)P_Y(y). \tag{C.27}$$

C.3.2. Continuous variables. If $\Omega_X = \mathbb{R}^n$ and $\Omega_Y = \mathbb{R}^m$, we can define the joint probability density $f_{XY}(\boldsymbol{x}, \boldsymbol{y})$ by

$$\boxed{\int_C f_X(\boldsymbol{x}, \boldsymbol{y}) d^n\boldsymbol{x} d^m\boldsymbol{y} = P[(X, Y) \in C].} \tag{C.28}$$

Then the marginal densities are

$$f_X(\boldsymbol{x}) \equiv \int f_{XY}(\boldsymbol{x}, \boldsymbol{y}) d^m\boldsymbol{y}, \qquad f_Y(\boldsymbol{y}) \equiv \int f_{XY}(\boldsymbol{x}, \boldsymbol{y}) d^n\boldsymbol{x}, \tag{C.29}$$

and (X, Y) are independent if and only if the joint density is separable in the sense of

$$f_{XY}(\boldsymbol{x}, \boldsymbol{y}) = f_X(\boldsymbol{x})f_Y(\boldsymbol{y}). \tag{C.30}$$

C.3.3. Independent and identically distributed (i.i.d.) variables. The construction of the joint probability space for multiple random variables is similar. In particular, n **independent and identically distributed (i.i.d.)** random variables $(X_1, \ldots, X_n) \in \Omega^n$ are defined as independent variables where each X_j has the same probability measure P. The joint probability measure is then the product measure

$$P_{X_1,\ldots,X_n} = \underbrace{P \otimes \cdots \otimes P}_{n \text{ terms}} \equiv P^{\otimes n}. \tag{C.31}$$

For example, if the random variables are discrete, then the joint probability distribution is

$$\boxed{P_{X_1,\ldots,X_n}(x_1, \ldots, x_n) \equiv P[(X_1 = x_1) \cap \cdots \cap (X_n = x_n)] = P(x_1) \ldots P(x_n).} \tag{C.32}$$

C.4. Conditioning

The probability $P[A|B]$ of an event A given that an event B has occurred is called a conditional probability. It is defined by

$$\boxed{P[A \cap B] = P[A|B]P[B].} \tag{C.33}$$

If $P[B] > 0$,

$$P[A|B] = \frac{P[A \cap B]}{P[B]}, \tag{C.34}$$

but if $P[B] = 0$, we must also have $P[A \cap B] = 0$ since $P[A \cap B] \leq P[B]$, and $P[A|B]$ conditioned on a zero-chance event B can be anything, although conventions exist depending on the problem.

Two events A and B are said to be **independent** if

$$\boxed{P[A \cap B] = P[A]P[B].} \tag{C.35}$$

Remark C.1. *Do not confuse independence with mutual exclusivity; there's no relation between the two concepts.*

Consider two random variables X and Y on the sample/event spaces $(\Omega_X \times \Omega_Y, F_X \otimes F_Y)$. For discrete random variables, the conditional probability distribution can be expressed in terms of the joint distribution defined by Eq. (C.25) as

$$\boxed{P_{X|Y}(x|y) \equiv P[X = x|Y = y] = \frac{P_{XY}(x,y)}{P_Y(y)} = \frac{P_{XY}(x,y)}{\sum_x (\text{numerator})}.} \tag{C.36}$$

If Y is continuous, conditioning becomes trickier, because $P[Y = \boldsymbol{y}]$ may be zero for all $\boldsymbol{y}$. Let $\Omega_Y = \mathbb{R}^m$. The way forward is the following [41]. Assume an event $B_\epsilon(\boldsymbol{y}) \in F_Y$ containing $\boldsymbol{y} \in \Omega_Y$ and possessing an m-dimensional volume ϵ, which should not depend on X. To define $P[X \in A|Y = \boldsymbol{y}]$, write the conditional probability in terms of $B_\epsilon(\boldsymbol{y})$ the usual way, then take the $\epsilon \to 0$ limit:

$$P[X \in A|Y = \boldsymbol{y}] \equiv \lim_{\epsilon \to 0} \frac{P\{(X \in A) \cap [Y \in B_\epsilon(\boldsymbol{y})]\}}{P[Y \in B_\epsilon(\boldsymbol{y})]}. \tag{C.37}$$

For example, consider the joint probability density defined by Eq. (C.28). For an infinitesimal ϵ,

$$P\{(X \in A) \cap [Y \in B_\epsilon(\boldsymbol{y})]\} = \epsilon \int_A f_{XY}(\boldsymbol{x}, \boldsymbol{y}) d^n\boldsymbol{x}, \quad P[Y \in B_\epsilon(\boldsymbol{y})] = \epsilon \int f_{XY}(\boldsymbol{x}, \boldsymbol{y}) d^n\boldsymbol{x} = \epsilon f_Y(\boldsymbol{y}), \tag{C.38}$$

where we can take ϵ out of the integrals because it is assumed to be independent of $\boldsymbol{x}$. The conditional probability becomes

$$P[X \in A|Y = y] = \frac{\int_A f_{XY}(\boldsymbol{x}, \boldsymbol{y}) d^n\boldsymbol{x}}{f_Y(\boldsymbol{y})}, \tag{C.39}$$

and the conditional density $f_{X|Y}(\boldsymbol{x}|\boldsymbol{y})$ becomes

$$\boxed{f_{X|Y}(\boldsymbol{x}|\boldsymbol{y}) = \frac{f_{XY}(\boldsymbol{x}, \boldsymbol{y})}{f_Y(\boldsymbol{y})} = \frac{f_{XY}(\boldsymbol{x}, \boldsymbol{y})}{\int (\text{numerator}) d^n\boldsymbol{x}}.} \tag{C.40}$$

Side note. *The so-called Borel-Kolmogorov paradox arises [41] if we assume that the volume of B_ϵ varies with $\boldsymbol{x}$, say, $\epsilon g(\boldsymbol{x})$. Then the limit would give us*

$$\frac{f_{XY}(\boldsymbol{x}, \boldsymbol{y}) g(\boldsymbol{x})}{\int (\textit{numerator}) d^n\boldsymbol{x}}, \tag{C.41}$$

which is arbitrary and depends on the $g(\boldsymbol{x})$ we choose. According to mathematicians, this paradox shows that conditioning on the outcome of a continuous variable is ill-defined, and the so-called disintegration theorem is needed to deal with it. Fortunately, Eq. (C.40) is correct afterall.

C.5. Conditional expectation

Given that $Y = y$ has occurred, the conditional expected value of X is written as $\mathbb{E}(X|Y = y)$. For example, if both X and Y are discrete, the conditional expectation is given by

$$\mathbb{E}(X|Y = y) = \sum_x x P_{X|Y}(x|y). \tag{C.42}$$

Notice that this is a function of y, so we can regard $\mathbb{E}(X|Y)$ **as a function of the random variable** Y. For example, suppose that Y is a binary random variable about whether it rains or not:

$$\text{no rain}: \quad Y = 0, \qquad\qquad \text{rain}: \quad Y = 1, \tag{C.43}$$

and X is the duration of a bus ride. Then

(1) $\mathbb{E}(X|Y = 0)$ is the expected duration given that there's no rain ($Y = 0$).
(2) $\mathbb{E}(X|Y = 1)$ is the expected duration given that there's rain ($Y = 1$).

$\mathbb{E}(X|Y)$ is a function of Y, so it is also a random variable.

Since $\mathbb{E}(X|Y)$ is another random variable as a function of Y, we can take its expectation again using the probability distribution of Y. For example, if both variables are discrete, we have

$$\mathbb{E}[\mathbb{E}(X|Y)] = \sum_y \left[\sum_x x P_{X|Y}(x|y)\right] P_Y(y) = \sum_{x,y} x P_{XY}(x, y) = \mathbb{E}(X). \tag{C.44}$$

In general,

$$\boxed{\mathbb{E}[\mathbb{E}(X|Y)] = \mathbb{E}(X)} \tag{C.45}$$

is called the **law of total expectation**, which in fact works for any types of random variables. We can use this to verify that Eq. (C.40) is the appropriate conditional density, not Eq. (C.41).

Exercise C.1. Derive the even more general law

$$\mathbb{E}\left\{b(Y)\,\mathbb{E}\left[a(X)|Y\right]\right\} = \mathbb{E}\left[b(Y)a(X)\right] \tag{C.46}$$

for any functions a and b, assuming discrete random variables. Verify that this holds for Eq. (C.40).

The **conditional variance** is given by

$$\mathbb{V}(X|Y = y) = \mathbb{E}(X^2|Y = y) - [\mathbb{E}(X|Y = y)]^2, \tag{C.47}$$

which is simply the variance of X given that we know $Y = y$. Since this is a function of $Y = y$, we can again regard $\mathbb{V}(X|Y)$ as a random variable that is a function of Y.

A useful law is the **law of total variance** (https://en.wikipedia.org/wiki/Law_of_total_variance):

$$\boxed{\mathbb{V}(X) = \mathbb{E}[\mathbb{V}(X|Y)] + \mathbb{V}[\mathbb{E}(X|Y)].} \tag{C.48}$$

(1) The first term $\mathbb{E}[\mathbb{V}(X|Y)]$ is obtained by first computing the variance of X conditioned on $Y = y$ using Eq. (C.47). Treating $\mathbb{V}(X|Y)$ as a function of Y, we then compute its expectation.
(2) The second term is $\mathbb{V}[\mathbb{E}(X|Y)]$ obtained by first computing $\mathbb{E}(X|Y = y)$ conditioned on $Y = y$. Treating $\mathbb{E}(X|Y)$ as a function of Y, we then compute its variance.

C.6. Gaussian random variables

A multivariate Gaussian random variable (also called normal random variable) with $\Omega = \mathbb{R}^n$ has the probability density

$$\boxed{f_X(\boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^n \det \Sigma}} \exp\left[-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{m})^\top \Sigma^{-1}(\boldsymbol{x} - \boldsymbol{m})\right],} \quad \boldsymbol{x} \in \mathbb{R}^n, \tag{C.49}$$

where $\boldsymbol{m}$ is the mean vector and Σ is the covariance matrix, defined as

$$\boxed{\mathbb{E}(X) = \boldsymbol{m},} \qquad \boxed{\mathrm{COV}(X_j, X_l) \equiv \mathbb{E}\left\{[X_j - \mathbb{E}(X_j)][X_l - \mathbb{E}(X_l)]\right\} = \Sigma_{jl}.} \tag{C.50}$$

We often write a vectoral Gaussian random variable using the shorthand

$$X \sim \mathcal{N}(\boldsymbol{m}, \Sigma). \tag{C.51}$$

Gaussian random variables have the following nice properties:

(1) Any linear combination of Gaussian random variables are also Gaussian random variables. To be specific, if we define

$$Y_j = \sum_l A_{jl} X_l + b_j, \tag{C.52}$$

where $\{A_{jl}\}$ and $\{b_j\}$ are real constants, then $\{Y_j\}$ are also Gaussian random variables. The means and covariances of the new random variables become

$$\mathbb{E}(Y_j) = \sum_l A_{jl}\,\mathbb{E}(X_l) + b_j, \qquad \mathrm{COV}(Y_j, Y_l) = \sum_{m,n} A_{jm}\Sigma_{mn}A_{ln}. \tag{C.53}$$

In matrix form, if we write $\Sigma_{jl}(Y) \equiv \mathrm{COV}(Y_j, Y_l)$, then

$$\mathbb{E}(Y) = A\boldsymbol{m} + \boldsymbol{b}, \qquad \Sigma(Y) = A\Sigma A^\top. \tag{C.54}$$

(2) A corollary is that, if we consider only l of the random variables, say,

$$X^{(1)} \equiv \begin{pmatrix} X_1 \\ \vdots \\ X_l \end{pmatrix}, \tag{C.55}$$

then its marginal probability density is still Gaussian and the means $\mathbb{E}(X_j)$ and covariances $\mathrm{COV}(X_j, X_k)$ remain unchanged, i.e.,

$$X^{(1)} \sim \mathcal{N}(\boldsymbol{m}^{(1)}, \Sigma^{(1)}), \tag{C.56}$$

where $\boldsymbol{m}^{(1)}$ is the first l entries of $\boldsymbol{m}$ and $\Sigma^{(1)}$ is the top-left $l \times l$ submatrix of Σ.

(3) If Σ is a diagonal matrix (i.e., the variables are all **uncorrelated**), then the Gaussian random variables are all **independent** from one another (i.e., $f_X(\boldsymbol{x})$ is separable into a product of n functions $\prod_j f_{X_j}(x_j)$, where each $f_{X_j}(x_j)$ is Gaussian.)

Remark C.2. *In general, independence always implies a diagonal covariance matrix, but the converse need not be true; Gaussian random variables are just special.*

(4) If Σ can be partitioned as

$$\Sigma = \begin{pmatrix} \Sigma^{(1)} & \\ & \Sigma^{(2)} \end{pmatrix}, \tag{C.57}$$

where $\Sigma^{(1)}$ is $l \times l$, $\Sigma^{(2)}$ is $(n-l) \times (n-l)$, and the rest of the entries are zero, then $f_X(\boldsymbol{x})$ can be factorized as

$$f_X(\boldsymbol{x}) = f_{X^{(1)}}(\boldsymbol{x}^{(1)}) f_{X^{(2)}}(\boldsymbol{x}^{(2)}), \tag{C.58}$$

$$X^{(1)} \equiv \begin{pmatrix} X_1 \\ \vdots \\ X_l \end{pmatrix}, \quad X^{(2)} \equiv \begin{pmatrix} X_{l+1} \\ \vdots \\ X_n \end{pmatrix}. \tag{C.59}$$

A fancier way of writing this fact is to use the direct sum $\oplus$ (see Sec. B.11). Instead of Eqs. (C.57) and (C.59), we can write

$$\Sigma = \Sigma^{(1)} \oplus \Sigma^{(2)}, \qquad X = X^{(1)} \oplus X^{(2)}, \tag{C.60}$$

where $\Sigma^{(1)}$ is the covariance matrix for $X^{(1)}$ and $\Sigma^{(2)}$ is the covariance matrix for $X^{(2)}$. $\Sigma = \Sigma^{(1)} \oplus \Sigma^{(2)}$ means that the covariance between any entry of $X^{(1)}$ and any entry of $X^{(2)}$ is zero. Then Eq. (C.58) holds.

The simplest case is when $n = 1$, and the probability density of $X \sim \mathcal{N}(m, \sigma^2)$ becomes

$$\boxed{f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-m)^2}{2\sigma^2}\right],} \tag{C.61}$$

where $\sigma \equiv \sqrt{\Sigma_{11}}$ is the standard deviation.

C.7. Poisson random variables

Let $\mathbb{N}_0 = \{0, 1, 2, \dots\}$ be the set of natural numbers and assume a sample space $\Omega = \mathbb{N}_0^J$, where each outcome $(N_1, N_2, \dots, N_J)$ is a set of J nonnegative integers. The Poisson distribution is defined as

$$\boxed{P_N(n_1, \dots, n_J) = \prod_{j=1}^{J} e^{-m_j} \frac{m_j^{n_j}}{n_j!}.} \tag{C.62}$$

$(N_1, N_2, \dots, N_J)$ are all independent from one another, and the mean and covariance are given by

$$\boxed{\mathbb{E}(N_j) = m_j,} \qquad \boxed{\mathrm{COV}(N_j, N_k) = m_j \delta_{jk}.} \tag{C.63}$$

We denote such a vectoral Poisson random variable as

$$N \sim \text{Poisson}(\boldsymbol{m}). \tag{C.64}$$

C.7.1. An origin of Poisson random variables*. There are a few ways that Poisson random variables arise. One way is the following:

(1) Perform M independent experiments, and label each experiment by $m = 1, \dots, M$. In each experiment, generate a binary random variable X_m with probability mass function

$$P[X_m = 0] = 1 - \epsilon, \qquad P[X_m = 1] = \epsilon. \tag{C.65}$$

For a concrete example, let M be the number of time slots over some time interval and X_m be the photon number arriving at some detectors during the mth time slot.

(2) If $X_m = 1$, generate a discrete random variable Y_m with probability mass function

$$P[Y_m = j] = p_j, \quad j = 1, \dots, J. \tag{C.66}$$

Continuing the earlier example, suppose that there are J detectors and $\{1, \dots, J\}$ are the labels of the detectors. If a photon arrives during the mth time slot ($X_m = 1$), it is detected by one of the detectors, Y_m is the label of that detector, and $P[Y_m = j] = p_j$ is the probability that the jth detector detects the photon.

(3) At the end of the M experiments, let L be the number of times X_m hits 1:

$$L \equiv \sum_{m=1}^{M} X_m, \tag{C.67}$$

and N_j be the number of times Y_m hits j:

$$N_j \equiv \sum_{m:X_m=1} \delta_{Y_m j}, \qquad L = \sum_{j=1}^{J} N_j. \tag{C.68}$$

In the earlier example, L is the total number of photons that are detected by all detectors and N_j is the total photon number detected by the jth detector.

(4) L is binomial:

$$P_L(l) = \binom{M}{l} \epsilon^l (1-\epsilon)^{M-l}. \tag{C.69}$$

In the limit of $\epsilon \to 0$, $M \to \infty$, and $M\epsilon$ staying fixed, L is a Poisson random variable with mean $\langle L \rangle = M\epsilon$ (https://en.wikipedia.org/wiki/Poisson_limit_theorem):

$$P_L(l) \to \exp(-\langle L \rangle) \frac{\langle L \rangle^l}{l!}. \tag{C.70}$$

(5) Conditioned on $L = l$, the probability distribution of N is multinomial (https://en.wikipedia.org/wiki/Multinomial_distribution):

$$P_{N|L}(n_1, \ldots, n_J | l) = \delta_{\sum_j n_j, l} \frac{l!}{n_1! \ldots n_J!} p_1^{n_1} \ldots p_J^{n_J}. \tag{C.71}$$

Assuming that L is Poisson, the marginal probability of N becomes Poisson:

$$P_N(n_1, \ldots, n_J) = \sum_{l=0}^{\infty} P_{N|L}(n_1, \ldots, n_J | l) P_L(l) = \sum_{l=0}^{\infty} e^{-\langle L \rangle} \frac{\langle L \rangle^l}{l!} \delta_{\sum_j n_j, l} \frac{l!}{n_1! \ldots n_J!} p_1^{n_1} \ldots p_J^{n_J} \tag{C.72}$$

$$= e^{-\langle L \rangle} \langle L \rangle^{\sum_j n_j} \frac{p_1^{n_1} \ldots p_J^{n_J}}{n_1! \ldots n_J!} \sum_{l=0}^{\infty} \delta_{\sum_j n_j, l} = \prod_{j=1}^{J} e^{-m_j} \frac{m_j^{n_j}}{n_j!}, \quad m_j = \langle L \rangle p_j. \tag{C.73}$$

C.7.2. Poisson process*. If each Y_m is not restricted to be a discrete random variable, we obtain a **Poisson process** in general. For each Y_m, let $\Omega_Y = \mathbb{R}^n$ be its sample space (generalizing $\{1, \ldots, J\}$), F_Y be its event space (a set of subsets of Ω_Y), and $p : F_Y \to [0, 1]$ be its probability measure (generalizing p_j). The Poisson process is now defined as a random measure $N(A)$, where $A \in F_Y$ is a subset of Ω_Y. Continuing the photon example, we now assume that $\Omega_Y = \mathbb{R}^2$ is the detector area. Then $A \in F_Y$ is a subset of Ω_Y, i.e., a smaller area on the detector, and $N(A)$ is the photon number detected on area A. The total number detected in the whole sample space Ω_Y is now $L \equiv N(\Omega_Y)$, and we write $\langle L \rangle \equiv \mathbb{E}(L)$ as before. The Poisson process obeys the following properties:

(1) $N(A)$ for any $A \in F_Y$ is a Poisson random variable with mean

$$\mathbb{E}[N(A)] = \langle L \rangle p(A). \tag{C.74}$$

(2) $N(A)$ and $N(B)$ are independent if $A \cap B = \varnothing$.

C.8. Random process*

A random process in the time domain is a randomly fluctuating function of time. The easiest way of modeling one is to assume discrete times

$$\mathcal{I} \equiv \{t_j = t_0 + j\Delta t : j = 1, 2, \ldots, J\} \tag{C.75}$$

and consider a set of random variables $(X(t_1), X(t_2), \ldots, X(t_J))$, each labeled by a time t_j. There are two ways of modeling them:

(1) Assume that there is an underlying probability space (Ω, F, P) with an abstract sample space Ω such that $X : \Omega \times \mathcal{I} \to \mathbb{R}^n$ is a function $X_\omega(t_j)$ of both an abstract variable $\omega \in \Omega$ in the sample space and a time $t_j \in \mathcal{I}$, producing a vector in $\mathbb{R}^n$.

(2) Assume that each $X(t_j)$ has a sample space $\Omega_j \subseteq \mathbb{R}^n$, so that the sample space of the whole process is $\Omega = \Omega_1 \times \cdots \times \Omega_J$ and there is an underlying probability measure P for $(X(t_1), X(t_2), \ldots, X(t_J))$.

There is not much difference between the two approaches in what follows.

With discrete time, there really isn't much difference between a random process and a vector of random variables. For simplicity, assume that each $X(t_j)$ is a real number, i.e., $\Omega_j \subseteq \mathbb{R}$. We can study its mean

$$\mathbb{E}\left[X(t_j)\right] \equiv m(t_j) \tag{C.76}$$

and the covariance matrix

$$\Sigma_{jk} \equiv \mathrm{COV}\left[X(t_j), X(t_k)\right] \equiv \mathbb{E}\left\{[X(t_j) - m(t_j)][X(t_k) - m(t_k)]\right\}, \tag{C.77}$$

just as we would for a vector of random variables.

C.8.1. Wide-sense stationary process. An additional assumption we often make in physics and engineering is that the covariance is a function of the time difference only:

$$\boxed{\mathrm{COV}\left[X(t_j), X(t_k)\right] = C(t_k - t_j),} \qquad C : \{-(J-1)\Delta t, \ldots, (J-1)\Delta t\} \to \mathbb{R}, \tag{C.78}$$

where C is a single-variable function. When the covariance matrix has this property, we say that the process is **wide-sense stationary**. The definition of strict stationarity is a bit more complicated (https://en.wikipedia.org/wiki/Stationary_process) and often unnecessary.

Since $t_k - t_j = (k-j)\Delta t$, each covariance-matrix entry Σ_{jk} depends on j and k only in terms of their difference $k - j$, i.e.,

$$\Sigma_{jk} = C(t_k - t_j) \equiv c_{k-j}, \tag{C.79}$$

and it looks like

$$\Sigma = \begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_{J-1} \\ c_{-1} & c_0 & c_1 & \cdots & c_{J-2} \\ c_{-2} & c_{-1} & c_0 & \cdots & c_{J-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_{-(J-1)} & c_{-(J-2)} & \cdots & c_{-1} & c_0 \end{pmatrix}. \tag{C.80}$$

A matrix is called Toeplitz if it has this form. Moreover, assume that $C(\tau)$ is periodic with

$$C(\tau) = C(\tau + T) \quad \forall \tau, \quad T \equiv J\Delta t. \tag{C.81}$$

This is a good approximation if $C(\tau)$ is concentrated near $\tau = 0$ and $C(\tau) \approx 0$ for τ near $\pm T/2$, i.e., $X(t_j)$ and $X(t_k)$ are uncorrelated if the time difference $|t_k - t_j|$ is close to half the duration of the process $T/2$, and T is very long so that we can ignore the covariance for $|t_k - t_j|$ beyond $T/2$. In other words, we assume that the entries of Σ decay to very small numbers as we move away from the diagonal, so that the periodic assumption is harmless. With the periodic C, c_l is periodic with period J, that is,

$$c_l = c_{l+J} \quad \forall l, \tag{C.82}$$

and Σ becomes a circulant matrix (https://en.wikipedia.org/wiki/Circulant_matrix), which looks like

$$\Sigma = \begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_{J-1} \\ c_{J-1} & c_0 & c_1 & \cdots & c_{J-2} \\ c_{J-2} & c_{J-1} & c_0 & \cdots & c_{J-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_1 & c_2 & \cdots & c_{J-1} & c_0 \end{pmatrix}. \tag{C.83}$$

A circulant matrix has the eigenvalue decomposition

$$\Sigma = UDU^\dagger, \qquad U_{jl} = \frac{1}{\sqrt{J}} \exp(-i\omega_l t_j), \qquad D_{lk} = \lambda_l \delta_{lk}, \qquad \omega_l = l\Delta\omega, \qquad \Delta\omega \equiv \frac{2\pi}{J\Delta t} = \frac{2\pi}{T}, \tag{C.84}$$

so that

$$\Sigma_{jk} = c_{k-j} = C(\tau_k) = \frac{1}{J} \sum_{l=l_0}^{l_0+J-1} \lambda_l \exp(-i\omega_l \tau_k), \quad \tau_k \equiv k\Delta t, \tag{C.85}$$

$$\lambda_l = \sum_{k=k_0}^{k_0+J-1} c_k \exp(i\omega_l \tau_k) = \sum_{k=k_0}^{k_0+J-1} C(\tau_k) \exp(i\omega_l \tau_k). \tag{C.86}$$

We may pick $l_0 = k_0 = -\lfloor J/2 \rfloor$, so that $\omega_l \in [-\pi/\Delta t, \pi/\Delta t)$ and $\tau_k \in [-T/2, T/2)$. The **power spectral density** of the process is defined in terms of the eigenvalues as

$$\boxed{S(\omega_l) \equiv \lambda_l \Delta t = \sum_{k=k_0}^{k_0+J-1} C(\tau_k) \exp(i\omega_l \tau_k) \Delta t.} \tag{C.87}$$

It is given by the Fourier transform of the covariance function $C(\tau)$. Since Σ is symmetric and positive-semidefinite ($\Sigma = \Sigma^\top$ and $u^\top \Sigma u \geq 0$ for all $u \in \mathbb{R}^n$), all its eigenvalues are nonnegative, and we have $\lambda_l \geq 0$ and $S(\omega_l) \geq 0$ for all l.

To measure the power spectral density in practice, consider the mean-subtracted process

$$Y(t_j) \equiv X(t_j) - m(t_j) \tag{C.88}$$

and write

$$S(\omega) = \sum_{k=0}^{J-1} \mathbb{E}\left[Y(t_j) Y(t_k)\right] \exp[i\omega(t_k - t_j)] \Delta t. \tag{C.89}$$

Notice that the left-hand side does not depend on t_j, so we can do

$$S(\omega) = \frac{1}{J} \sum_{j=0}^{J-1} S(\omega) = \frac{1}{T} \sum_{j,k} \mathbb{E}\left[Y(t_j) Y(t_k)\right] \exp[i\omega(t_k - t_j)] \Delta t^2 = \frac{1}{T} \mathbb{E}\left[\left|\tilde{Y}_T(\omega)\right|^2\right], \tag{C.90}$$

where

$$\tilde{Y}_T(\omega) \equiv \sum_{k=0}^{J-1} Y(t_k) \exp(i\omega t_k) \Delta t \tag{C.91}$$

is the Fourier transform of the process Y. If we measure $|\tilde{Y}_T(\omega)|^2/T$ repeatedly and take the average of the observations, it should converge to the expected value $S(\omega)$. Under a further assumption about the random process called ergodicity, we can also obtain $S(\omega)$ by the long-time limit

$$\lim_{T \to \infty} \frac{1}{T} \left|\tilde{Y}_T(\omega)\right|^2 = S(\omega). \tag{C.92}$$

C.8.2. Continuous-time limit. We now take the limit $\Delta t \to 0$ with finite $T \equiv J \Delta t$. The frequencies ω_l are still discrete with spacing

$$\Delta\omega = \frac{2\pi}{T}, \tag{C.93}$$

but now they go from $-\infty$ to ∞. We should define the continuous Fourier transform as

$$\tilde{Y}_T(\omega_l) \equiv \int_{t_0}^{t_0+T} Y(t) \exp(i\omega_l t) dt. \tag{C.94}$$

The power spectral density becomes

$$S(\omega_l) = \int_{-T/2}^{T/2} C(\tau) \exp(i\omega_l \tau) d\tau = \frac{1}{T} \mathbb{E}\left[\left|\tilde{Y}_T(\omega_l)\right|^2\right]. \tag{C.95}$$

C.8.3. Continuous-frequency limit. If we keep Δt nonzero but take $J \to \infty$, so that time goes from $-\infty$ to ∞, then the frequency becomes continuous with $\Delta\omega = \pi/J\Delta t \to 0$ but still stays in the range

$$\omega \in [-\pi/\Delta t, \pi/\Delta t). \tag{C.96}$$

and we write

$$S(\omega) = \sum_{k=-\infty}^{\infty} C(\tau_k) \exp(i\omega\tau_k) \Delta t = \lim_{T \to \infty} \frac{1}{T} \mathbb{E}\left[\left|\tilde{Y}_T(\omega)\right|^2\right]. \tag{C.97}$$

C.8.4. White noise. If a wide-sense-stationary zero-mean process $Y(t)$ is uncorrelated at different times, then we can assume

$$\mathbb{E}\left[Y(t_j)Y(t_k)\right] = s\frac{\delta_{jk}}{\Delta t}, \qquad S(\omega_l) = s. \tag{C.98}$$

We call Y a white noise because the power spectral density is constant. If the sequence $\{Y(t_1), Y(t_2), \dots\}$ is also normal, i.e., $Y \sim \mathcal{N}(0, \Sigma)$, then we call Y a Gaussian white noise. In the continuous-time limit, we write

$$\mathbb{E}\left[Y(t)Y(t')\right] = s\delta(t - t'), \tag{C.99}$$

where δ is the Dirac delta.

An important example of white noise occurs when we measure a stream of pulses in a coherent state with constant photon flux. The mean photon number in each pulse is the infinitesimal $|\alpha_j|^2 = r\Delta t$, where r is the finite mean photon flux (mean number per second), so the mean of a quadrature must scale as $\sqrt{2}\,\mathrm{Re}(\alpha e^{-i\theta}) \propto \sqrt{\Delta t}$, while the variance is $1/2$ regardless of Δt. Each homodyne output X_j is then a Gaussian random variable with

$$\mathbb{E}\left(X_j\right) \propto \sqrt{\Delta t}, \qquad \mathrm{COV}(X_j, X_k) = \frac{1}{2}\delta_{jk}. \tag{C.100}$$

If we divide X_j by $\sqrt{\Delta t}$, then the process becomes a signal plus a Gaussian white noise.

If we perform photon counting, on the other hand, the process is Poisson with

$$\mathbb{E}(N_j) = r\Delta t, \qquad \mathrm{COV}(N_j, N_k) = \delta_{jk}\,\mathbb{E}(N_j) = r\delta_{jk}\Delta t. \tag{C.101}$$

Then $[N_j - \mathbb{E}(N_j)]/\Delta t$ is also a white noise with power spectral density $S(\omega) = s = r$.

C.8.5. Wiener process. Let Y be a Gaussian white noise and define another random process W by the sum

$$W(t_0) = 0, \qquad W(t_j) = W(t_{j-1}) + Y(t_j)\Delta t = \sum_{k=1}^{j} Y(t_k)\Delta t. \tag{C.102}$$

In the continuous-time limit, W is called a Wiener process, also called a Brownian motion. We may think of $W(t)$ as a process whose rate of change is driven by white noise:

$$\frac{dW(t)}{dt} = Y(t), \qquad W(t) = \int_0^t Y(\tau)d\tau. \tag{C.103}$$

The covariance of W is

$$\mathbb{E}\left[W(t_j)W(t_k)\right] = s\min\left\{t_j, t_k\right\}. \tag{C.104}$$

In particular, the variance $\mathbb{E}\left[W(t)^2\right] = st$ grows linearly with time, as one expects from a Brownian motion. Note that the Wiener process is not stationary in any sense.

Remark C.3. *Beware that the variance of the white noise $\mathbb{E}[Y(t_j)^2] = s/\Delta t$ scales inversely with Δt and becomes infinite in the continuous limit $\Delta t \to 0$. This means that we can't assume $Y(t)$ to be an ordinary function in a differential equation and ordinary calculus becomes questionable because of the infinite variance. It turns out that one should use a new calculus called stochastic calculus (https://en.wikipedia.org/wiki/Stochastic_calculus) to deal with white noise. In our poor-man's approach to random processes, we just stick with discrete time and take the $\Delta t \to 0$ limit when it looks safe to do so.*

Side note. *Mathematicians prefer to work with the Wiener process and not the white noise directly because they hate the Dirac delta. In physics and engineering, the white noise is a more intuitive object as it models what we observe in measurements.*

C.9. Abstract measure theory*

Mathematicians often prefer to use abstract measure theory to study probability. While mostly unnecessary for physicists, it is useful to learn at least the notation so that we can read their literature. The notation is also quite elegant as we no longer need to write different expressions for discrete and continuous variables.

C.9.1. Lebesgue integral. Given a measure P on (Ω, F), where Ω is an abstract sample space and F is a σ-algebra of Ω (a set of subsets of Ω that satisfy certain properties to make mathematicians happy), the Lebesgue integral of a function $g : \Omega \to \mathbb{R}$ is written as

$$\int g(x)dP(x). \tag{C.105}$$

Think of $dP(x)$ as the amount of certain stuff in a tiny region of Ω around x, and $\int$ as a fancy way of writing a sum over all the tiny regions that comprise Ω. If we'd like to integrate over a subset $A \in F$ only, then we can write

$$\int_{x\in A} g(x)dP(x) = \int [x \in A]g(x)dP(x), \tag{C.106}$$

where

$$[\text{statement}] \equiv \begin{cases} 1, & \text{if the statement is true,} \\ 0, & \text{otherwise} \end{cases} \tag{C.107}$$

is called the Iversen bracket. $[x \in A]$ is also called the indicator function in measure theory.

If P is a probability measure, think of $dP(x)$ as the probability that the outcome is in a tiny region around x. The expectation of a random variable is given by

$$\mathbb{E}(g) = \int g(x)dP(x), \tag{C.108}$$

while the probability of an event $A \in F$ can be written as

$$P[A] = \int_{x\in A} dP(x) = \int [x \in A]dP(x). \tag{C.109}$$

If the sample space is countable, the Lebesgue integral gives

$$\mathbb{E}(g) = \sum_x g(x)P(x), \qquad P[A] = \sum_{x\in A} P(x). \tag{C.110}$$

If $\Omega \subseteq \mathbb{R}^n$, we use the conventional probability density f to write

$$\mathbb{E}(g) = \int g(x)f(x)d^n x, \qquad P[A] = \int_{x\in A} f(x)d^n x. \tag{C.111}$$

In other words, just replace $dP(x)$ by $P(x)$ and $\int_{x\in A}$ by $\sum_{x\in A}$ in the discrete case and replace $dP(x)$ by $f(x)d^n x$ in the continuous case.

C.9.2. Lebesgue measure. The Lebesgue measure for $\Omega \subseteq \mathbb{R}^n$ is simply a fancy name for a measure that gives back our ordinary n-dimensional integral:

$$\int g(x)dP(x) = \int g(x)d^n x. \tag{C.112}$$

In other words, $dP(x) = d^n x$ for a Lebesgue measure is the volume of a tiny n-dimensional cube around x.

Remark C.4. *The Lebesgue integral is a general concept for any measure P, whereas the Lebesgue measure is a special type of measure that gives us back an ordinary integral. Both are named after Lebesgue but they are different concepts.*

C.9.3. Radon-Nikodym derivative. The Radon-Nikodym derivative generalizes the concept of the density function. Let P and Q be two measures on the same (Ω, F). The Radon-Nikodym derivative of P with respect to Q, written as $\frac{dP}{dQ}(x)$, is defined by

$$\int g(x)dP(x) = \int g(x)\frac{dP}{dQ}(x)dQ(x) \tag{C.113}$$

for any function g. In other words, it allows us to substitute an integral of g with respect to P with an integral of gdP/dQ with respect to Q. The derivative exists if and only if

$$P(A) \neq 0 \text{ implies } Q(A) \neq 0 \quad \forall A \in F. \tag{C.114}$$

We say that Q dominates P, written in brief as $P \ll Q$, under this condition. People also say that P is "absolutely continuous" with respect to Q.

dP/dQ is called a derivative mainly because the notation looks like one; its relations with all the other derivatives in calculus are rather tenuous. We should think of it simply as a ratio $dP(x)/dQ(x)$ between the two amounts of stuffs in the same region around x. We need Q to dominate P for the ratio to be well defined because we need $dQ(x) \neq 0$ whenever $dP(x) \neq 0$.

If P is a probability measure and Q is a standard measure for (Ω, F), e.g., the Lebesgue measure, then dP/dQ is called a probability density. If P and Q are both probability measures, dP/dQ often arises in statistics, where it is called the likelihood ratio.

Examples:

(1) If Ω is countable, then

$$\int g(x)dP(x) = \sum_x g(x)P(x) = \sum_x g(x)\frac{P(x)}{Q(x)}Q(x), \qquad \frac{dP}{dQ}(x) = \frac{P(x)}{Q(x)}. \tag{C.115}$$

We see in this case why we need Q to dominate P: we need $P(x)/Q(x) < \infty$ for all $x \in \operatorname{support} P \equiv \{x \in \Omega : P(x) > 0\}$ so we need $\operatorname{support} P \subseteq \operatorname{support} Q$.

In particular, if Q is the counting measure such that $Q(x) = 1$ for all x, then $P(x)$ is its own Radon-Nikodym derivative.

(2) For $\Omega \subseteq \mathbb{R}^n$, the conventional probability density $f(x)$ is the Radon-Nikodym derivative with respect to the Lebesgue measure, and we write $dQ(x) = d^n x$ and $dP(x) = f(x)d^n x$.

(3) If $P \ll Q \ll \sigma$, then dP/dQ is the ratio of the two Radon-Nikodym derivatives $(dP/d\sigma)(x)$ and $(dQ/d\sigma)(x)$:

$$\frac{dP}{dQ}(x) = \frac{\frac{dP}{d\sigma}(x)}{\frac{dQ}{d\sigma}(x)}. \tag{C.116}$$

For example, if σ is the Lebesgue measure ($d\sigma(x) = d^n x$) and $dP/d\sigma = f$ and $dQ/d\sigma = g$, then

$$\frac{dP}{dQ}(x) = \frac{f(x)}{g(x)}. \tag{C.117}$$

APPENDIX D

Quantum Mechanics

D.1. Schrödinger picture

This chapter will assume a **closed** quantum system throughout, i.e., a collection of stuff that doesn't interact with anything else. The **state** of the system is modeled by a vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}$ (see Appendix B for the math and notation). By convention, the norm of the vector should be equal to 1, viz.,

$$\boxed{\sqrt{\langle\psi|\psi\rangle} = 1.} \tag{D.1}$$

The dynamics of the system is governed by a Hamiltonian operator $\hat{H}$, which is Hermitian ($\hat{H} = \hat{H}^\dagger$). Then we can define a unitary operator as

$$\boxed{\hat{U}(t) \equiv \exp\Big(-i\hat{H}t\Big),} \tag{D.2}$$

where $t \in \mathbb{R}$ is the time variable and I've redefined the Hamiltonian $\hat{H}$ so that $\hbar$ is absorbed into the new definition and doesn't appear in the formulas, for brevity. In the **Schrödinger picture**, the state evolves in time and becomes

$$\boxed{|\psi(t)\rangle = \hat{U}(t)\,|\psi\rangle} \tag{D.3}$$

after time t.

Exercise D.1. Prove that the quantum state remains normalized after any time t in the Schrödinger picture, viz., $\langle\psi(t)|\psi(t)\rangle = 1$ for any t.

Exercise D.2. Derive the Schrödinger equation

$$\frac{d\,|\psi(t)\rangle}{dt} = -i\hat{H}\,|\psi(t)\rangle\,. \tag{D.4}$$

D.2. Born's rule

D.2.1. Simple measurement. The simplest kind of quantum measurement is modeled by an orthonormal basis $\{|e_n\rangle : n = 1, \ldots, N\}$ of the Hilbert space $\mathcal{H}$. The set of possible outcomes are denoted by $n = 1, \ldots, N$, and the probability of observing a certain outcome n with this simple measurement at time t is assumed to be given by

$$\boxed{P(n) = |\,\langle e_n|\psi(t)\rangle\,|^2,} \tag{D.5}$$

where $|\psi(t)\rangle$ is the quantum state at time t in the Schrödinger picture. This rule of assigning probabilities to a quantum measurement is called Born's rule. It gives an operational meaning to the quantum state $|\psi(t)\rangle$.

D.2.2. von Neumann measurement. A Hermitian operator $\hat{A}$ is often called an **observable** in quantum mechanics. Any observable $\hat{A}$ on a finite-dimensional Hilbert space can be expressed in the diagonal form

$$\hat{A} = \sum_n \lambda_n\,|e_n\rangle\,\langle e_n|\,, \tag{D.6}$$

where each $|e_n\rangle$ is an eigenvector of $\hat{A}$ with eigenvalue λ_n, all the eigenvalues are real (because $\hat{A}$ is Hermitian), and $\{|e_n\rangle\}$ is an orthonormal basis of the Hilbert space $\mathcal{H}$. We say that a **von Neumann measurement** of the observable $\hat{A}$ is performed when the measurement outcome is a random variable with the set of all possible outcomes given

by the set of eigenvalues $\{\lambda_n\}$. If the eigenvalues are all different from one another (i.e., nondegenerate), then the probability of observing a certain eigenvalue λ_n in a von Neumann measurement is given by Born's rule

$$P[A = \lambda_n] = |\langle e_n|\psi(t)\rangle|^2. \tag{D.7}$$

If there may be multiple eigenvectors with the same eignvalue (degenerate eigenvalues), then we have to be more careful: the probability of observing a given eigenvalue λ is

$$\boxed{P[A = \lambda] = \sum_{n:\lambda_n=\lambda} |\langle e_n|\psi(t)\rangle|^2,} \tag{D.8}$$

i.e., we need to sum all the probabilities for outcomes that give the same eigenvalue $\lambda_n = \lambda$.

Side note. *In reality, a measurement is performed by a measurement apparatus (your eyes, a cat, a camera, photodetectors, etc.), and the laws of quantum measurement don't tell us what exactly counts as a measurement apparatus, why we have a separate rule for the measurement apparatus, and why we don't model it using quantum mechanics as well. This ambiguity is called the* ***measurement problem*** *in quantum mechanics. There are various interpretations of a quantum measurement but we won't touch that topic—in quantum optics, measurements are usually performed with photodetectors, and it's quite clear that those are the measurement devices that obey Born's rule in principle.*

Side note. *In quantum optics, measurements are usually performed with photodetectors, which absorb the light and convert it to energy excitations in the matter. Such measurements are called destructive. In this book, we do not consider nondestructive measurements and what happens to the quantum state post-measurement.*

Side note. *Another thing to note is that the probability distribution of a measurement outcome in an experiment is never exactly given by Born's rule; there will always be extra noise due to technical imperfections, e.g., thermal noise in detectors and circuits. The "quantum noise" due to Born's rule is often a tiny fraction of the total noise in a device.*

Exercise D.3. Prove that a measurement modeled by an orthonormal basis $\{|e_n\rangle\}$ satisfies the normalization condition

$$\sum_n P(n) = \sum_n |\langle e_n|\psi(t)\rangle|^2 = 1. \tag{D.9}$$

Exercise D.4. Prove that the **expected value** of the measurement outcome for a von Neumann measurement of $\hat{A}$ is given by

$$\boxed{\langle A\rangle \equiv \langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle\,.} \tag{D.10}$$

Prove that the **variance** of the measurement outcome is given by

$$\boxed{\left\langle \Delta A^2\right\rangle \equiv \langle\psi(t)|\left(\hat{A} - \langle A\rangle\right)^2|\psi(t)\rangle = \langle\psi(t)|\,\hat{A}^2\,|\psi(t)\rangle - \left[\langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle\right]^2.} \tag{D.11}$$

These are handy formulas in case we need the mean and variance only, not the full probability distribution.

D.2.3. Measurement of compatible observables. Suppose that two Hermitian operators $\hat{A}$ and $\hat{B}$ commute, i.e.,

$$\left[\hat{A}, \hat{B}\right] = 0. \tag{D.12}$$

We say that the two observables are compatible. Linear algebra says that there exists an orthonormal basis $\{|e_n\rangle\}$ such that $\hat{A}$ and $\hat{B}$ can both be expressed in the diagonal form

$$\hat{A} = \sum_n \lambda_n\,|e_n\rangle\,\langle e_n|\,, \qquad\qquad \hat{B} = \sum_n \lambda'_n\,|e_n\rangle\,\langle e_n|\,, \tag{D.13}$$

using the same basis. $\{|e_n\rangle\}$ are eigenvectors of both $\hat{A}$ and $\hat{B}$, λ_n is the eigenvalue of $\hat{A}$ associated with $|e_n\rangle$, while λ'_n is the eigenvalue of $\hat{B}$ associated with $|e_n\rangle$. If we perform a simple measurement with respect to this basis, we can write a joint probability distribution as

$$\boxed{P\big[A=\lambda \text{ and } B=\lambda'\big] = \sum_{n:\lambda_n=\lambda \text{ and } \lambda'_n=\lambda'} |\,\langle e_n|\psi(t)\rangle\,|^2.} \tag{D.14}$$

Another way of saying this is that compatible observables can be measured simultaneously using one simple measurement.

D.2.4. Continuous variables. For an infinite-dimensional Hilbert space, sometimes the diagonal form of an observable is an integral

$$\hat{A} = \int_{-\infty}^{\infty} \lambda\,|A=\lambda\rangle\,\langle A=\lambda|\,d\lambda, \tag{D.15}$$

where $\{|A=\lambda\rangle : \lambda\in\mathbb{R}\}$ are the orthonormal eigenvectors of $\hat{A}$ in the sense of

$$\hat{A}\,|A=\lambda\rangle = \lambda\,|A=\lambda\rangle\,, \qquad\qquad \big\langle A=\lambda\big|A=\lambda'\big\rangle = \delta(\lambda-\lambda'), \tag{D.16}$$

as introduced by Dirac. The completeness condition for $\{|A=\lambda\rangle\}$ can now be expressed as

$$\hat{I} = \int_{-\infty}^{\infty} |A=\lambda\rangle\,\langle A=\lambda|\,d\lambda. \tag{D.17}$$

The outcome of a von Neumann measurement of $\hat{A}$ is then a **continuous** random variable, the set of all possible outcomes is $\mathbb{R}$, and the probability density is

$$f_A(\lambda) = |\langle A=\lambda|\psi(t)\rangle|^2, \tag{D.18}$$

which is a variation of Born's rule. Remember the definition of a probability density: $f_A(\lambda)d\lambda$ is the probability of observing the outcome within the infinitesimal interval $[\lambda, \lambda+d\lambda)$.

Definition D.1. *For brevity, I call the distribution $P[A=\lambda]$ or $f_A(\lambda)$ that arises from a von Neumann measurement of $\hat{A}$* ***the probability distribution of*** *$\hat{A}$.*

Exercise D.5. Prove the normalization condition

$$\int_{-\infty}^{\infty} f_A(\lambda)d\lambda = 1 \tag{D.19}$$

if $f_A(\lambda)$ is given by Eq. (D.18).

Exercise D.6. Let $\hat{A}$ be an observable and its orthonormal eigenstates be $\{|A=\lambda\rangle : \lambda\in\mathbb{R}\}$, so that

$$\hat{A}\,|A=\lambda\rangle = \lambda\,|A=\lambda\rangle\,, \qquad \big\langle A=\lambda\big|A=\lambda'\big\rangle = \delta(\lambda-\lambda'), \qquad \int_{-\infty}^{\infty} |A=\lambda\rangle\,\langle A=\lambda|\,d\lambda = \hat{I}. \tag{D.20}$$

Define another observable $\hat{B}$ in terms of $\hat{A}$ as

$$\hat{B} \equiv a\hat{A} + b, \tag{D.21}$$

where a is a nonzero real c-number and b is a real c-number.

(1) Find the orthonormal eigenstates $\{|B=u\rangle : u\in\mathbb{R}\}$ of $\hat{B}$ in terms of $|A=\lambda\rangle$ so that they also satisfy

$$\hat{B}\,|B=u\rangle = u\,|B=u\rangle\,, \qquad \big\langle B=u\big|B=u'\big\rangle = \delta(u-u'), \qquad \int_{-\infty}^{\infty} |B=u\rangle\,\langle B=u|\,du = \hat{I}. \tag{D.22}$$

Answer:

$$|B=u\rangle = \frac{e^{i\theta}}{\sqrt{|a|}}\left|A=\frac{u-b}{a}\right\rangle, \tag{D.23}$$

where θ can be any real number; harmless to set $\theta=0$.

(2) If the probability density of $\hat{A}$ is $f_A(\lambda)$, find the probability density $f_B(u)$ of $\hat{B}$ in terms of f_A.
Answer:

$$f_B(u) = \frac{1}{|a|} f_A\left(\frac{u-b}{a}\right). \tag{D.24}$$

The $1/|a|$ factor in front is needed so that f_B remains normalized as $\int_{-\infty}^{\infty} f_B(u)du = 1$.

D.3. Heisenberg picture

Consider a simple measurement with respect to an orthonormal basis $\{|e_n\rangle : n = 1, \ldots, N\}$. In the Schrödinger picture, the probability of each outcome n is

$$P(n) = |\langle e_n|\psi(t)\rangle|^2 = \left|\langle e_n| \hat{U}(t) |\psi\rangle\right|^2 = \langle\psi| \hat{U}^\dagger(t) |e_n\rangle \langle e_n| \hat{U}(t) |\psi\rangle . \tag{D.25}$$

We can also compute this probability using the **Heisenberg picture** instead. Define

$$\hat{A}_n \equiv |e_n\rangle \langle e_n| . \tag{D.26}$$

Then the Heisenberg picture of $\hat{A}_n$ at time t is

$$\hat{A}_n(t) \equiv \hat{U}^\dagger(t)\hat{A}_n\hat{U}(t) = \hat{U}^\dagger(t) |e_n\rangle \langle e_n| \hat{U}(t). \tag{D.27}$$

It follows that the probability of observing n is

$$P(n) = \langle\psi| \hat{U}^\dagger(t) |e_n\rangle \langle e_n| \hat{U}(t) |\psi\rangle = \langle\psi| \hat{A}_n(t) |\psi\rangle . \tag{D.28}$$

The Heisenberg picture is convenient if $\hat{A}_n(t)$ is easier to compute than $|\psi(t)\rangle$.

Exercise D.7. Given an operator $\hat{A}$, the Heisenberg picture of $\hat{A}$ is defined as

$$\boxed{\hat{A}(t) \equiv \hat{U}^\dagger(t)\hat{A}\hat{U}(t),} \tag{D.29}$$

where $\hat{U}(t)$ is given by Eq. (D.2). Show that it obeys the Heisenberg equation of motion

$$\frac{d\hat{A}(t)}{dt} = -i\Big[\hat{A}(t), \hat{H}\Big]. \tag{D.30}$$

Exercise D.8. Following Exercise D.4, show that the expected value and variance of the outcome for a von Neumann measurement of $\hat{A}$ are given by

$$\boxed{\langle A\rangle = \langle\psi| \hat{A}(t) |\psi\rangle ,} \qquad \boxed{\left\langle \Delta A^2\right\rangle = \langle\psi| [\hat{A}(t)]^2 |\psi\rangle - \Big[\langle\psi| \hat{A}(t) |\psi\rangle\Big]^2,} \tag{D.31}$$

where $\hat{A}(t)$ is the Heisenberg picture of $\hat{A}$ at time t.

D.4. Interaction picture

Suppose that the Hamiltonian is the sum of two terms:

$$\hat{H} = \hat{H}_{\text{easy}} + \hat{\eta}. \tag{D.32}$$

It is often the case that the dynamics governed by $\hat{H}_{\text{easy}}$ is simple to solve. For example, we often assume that $\hat{H}_{\text{easy}}$ is the Hamiltonian of free EM fields and free matter, while $\hat{\eta}$ is the Hamiltonian that models their interaction. Let

$$\boxed{\hat{U}_{\text{easy}}(t) \equiv \exp\Big(-i\hat{H}_{\text{easy}}t\Big),} \tag{D.33}$$

which is the unitary with respect to $\hat{H}_{\text{easy}}$ alone. The central identity of the interaction picture is

$$\boxed{\hat{U}_I(t) \equiv \hat{U}^\dagger_{\text{easy}}(t)\hat{U}(t) = \mathcal{T}\exp\left[-i\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau\right],} \tag{D.34}$$

$$\boxed{\hat{\eta}_{\text{easy}}(\tau) \equiv \hat{U}^\dagger_{\text{easy}}(\tau)\hat{\eta}\hat{U}_{\text{easy}}(\tau),} \tag{D.35}$$

where $\mathcal{T}\exp$ is called the time-ordered exponential (https://en.wikipedia.org/wiki/Ordered_exponential), defined as

$$\begin{aligned}&\mathcal{T}\exp\left[-i\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau\right]\\ &\equiv \lim_{\Delta t\to 0}\exp\big[-i\hat{\eta}_{\text{easy}}(t)\Delta t\big]\exp\big[-i\hat{\eta}_{\text{easy}}(t-\Delta t)\Delta t\big]\ldots\exp\big[-i\hat{\eta}_{\text{easy}}(2\Delta t)\Delta t\big]\exp\big[-i\hat{\eta}_{\text{easy}}(\Delta t)\Delta t\big],\end{aligned} \tag{D.36}$$

and $\hat{\eta}_{\text{easy}}(\tau)$ is called the interaction picture of $\hat{\eta}$ (which is the Heisenberg picture of $\hat{\eta}$ using $\hat{U}_{\text{easy}}$). Now the expected value of any observable $\hat{A}$ can be expressed as

$$\langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle = \langle\psi|\,\hat{U}^\dagger(t)\hat{A}\hat{U}(t)\,|\psi\rangle = \langle\psi|\,\hat{U}^\dagger(t)\hat{U}_{\text{easy}}(t)\hat{U}^\dagger_{\text{easy}}(t)\hat{A}\hat{U}_{\text{easy}}(t)\hat{U}^\dagger_{\text{easy}}(t)\hat{U}(t)\,|\psi\rangle \tag{D.37}$$

$$= \boxed{\langle\psi|\,\hat{U}^\dagger_I(t)\hat{A}_{\text{easy}}(t)\hat{U}_I(t)\,|\psi\rangle\,,} \tag{D.38}$$

where

$$\hat{A}_{\text{easy}}(t) \equiv \hat{U}^\dagger_{\text{easy}}(t)\hat{A}\hat{U}_{\text{easy}}(t). \tag{D.39}$$

The main reason we use the interaction picture is that the interaction-picture operator $\hat{U}^\dagger_{\text{easy}}(\ldots)\hat{U}_{\text{easy}}$ is often simple to compute, so $\hat{\eta}_{\text{easy}}(t)$, $\hat{U}_I(t)$, and $\hat{A}_{\text{easy}}(t)$ are often easier to compute.

D.4.1. Derivation of Eq. (D.34). Assume the more general case where $\hat{H}_{\text{easy}}(t)$ and $\hat{\eta}(t)$ are time-dependent and write each unitary as a product of exponentials with tiny time step Δt:

$$\hat{U}(t) \equiv \mathcal{T}\exp\left\{-i\int_0^t [\hat{H}_{\text{easy}}(\tau)+\hat{\eta}(\tau)]d\tau\right\} \tag{D.40}$$

$$\begin{aligned}&\approx \exp[-i\hat{\eta}(t)\Delta t]\exp\left[-i\hat{H}_{\text{easy}}(t)\Delta t\right]\exp[-i\hat{\eta}(t-\Delta t)\Delta t]\exp\left[-i\hat{H}_{\text{easy}}(t-\Delta t)\Delta t\right]\\ &\quad\ldots\exp[-i\hat{\eta}(2\Delta t)\Delta t]\exp\left[-i\hat{H}_{\text{easy}}(2\Delta t)\Delta t\right]\exp[-i\hat{\eta}(\Delta t)\Delta t]\exp\left[-i\hat{H}_{\text{easy}}(\Delta t)\Delta t\right],\end{aligned} \tag{D.41}$$

$$\hat{U}_{\text{easy}}(t) \equiv \mathcal{T}\exp\left\{-i\int_0^t \hat{H}_{\text{easy}}(\tau)d\tau\right\} \tag{D.42}$$

$$\approx \exp\left[-i\hat{H}_{\text{easy}}(t)\Delta t\right]\exp\left[-i\hat{H}_{\text{easy}}(t-\Delta t)\Delta t\right]\ldots\exp\left[-i\hat{H}_{\text{easy}}(2\Delta t)\Delta t\right]\exp\left[-i\hat{H}_{\text{easy}}(\Delta t)\Delta t\right]. \tag{D.43}$$

Now the trick is to use Eq. (D.43) to write

$$\exp\left[-i\hat{H}_{\text{easy}}(\tau)\Delta t\right] = \hat{U}_{\text{easy}}(\tau)\hat{U}^\dagger_{\text{easy}}(\tau-\Delta t), \tag{D.44}$$

and then substitute this into Eq. (D.41), so that

$$\hat{U}^\dagger_{\text{easy}}(t)\hat{U}(t) \approx \underbrace{\hat{U}^\dagger_{\text{easy}}(t)\exp[-i\hat{\eta}(t)\Delta t]\hat{U}_{\text{easy}}(t)}_{\exp[-i\hat{\eta}_{\text{easy}}(t)\Delta t]}\underbrace{\hat{U}^\dagger_{\text{easy}}(t-\Delta t)\exp[-i\hat{\eta}(t-\Delta t)\Delta t]\hat{U}_{\text{easy}}(t-\Delta t)}_{\exp[-i\hat{\eta}_{\text{easy}}(t-\Delta t)\Delta t]}\hat{U}^\dagger_{\text{easy}}(t-2\Delta t)$$

$$\ldots\hat{U}_{\text{easy}}(2\Delta t)\hat{U}^\dagger_{\text{easy}}(\Delta t)\exp[-i\hat{\eta}(\Delta t)\Delta t]\hat{U}_{\text{easy}}(\Delta t) \tag{D.45}$$

$$= \exp\left[-i\hat{\eta}_{\text{easy}}(t)\Delta t\right]\exp\left[-i\hat{\eta}_{\text{easy}}(t-\Delta t)\Delta t\right]\ldots\exp\left[-i\hat{\eta}_{\text{easy}}(\Delta t)\Delta t\right] \tag{D.46}$$

$$\to \mathcal{T}\exp\left[-i\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau\right]. \tag{D.47}$$

D.5. Rotating-wave approximation

When using the interaction picture, we often encounter terms that oscillate in time as $\exp(-i\omega t)$:

$$\hat{\eta}_{\text{easy}}(t) = \cdots + (\ldots)\exp(-i\omega t) + \ldots \tag{D.48}$$

where ω is a positive or negative number. In the so-called rotating-wave approximation, we throw away such terms and keep only terms that remain constant in time. To see the rationale, consider the first-order perturbation of the interaction-picture unitary $\hat{U}_I(t)$ given by Eq. (D.34):

$$\hat{U}_I(t) \approx \hat{I} - i\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau. \tag{D.49}$$

The first-order term is an integral of $\hat{\eta}_{\text{easy}}(\tau)$ in time, and the integral of the oscillating term becomes

$$\int_0^t \hat{\eta}_{\text{easy}}(\tau)d\tau = \int_0^t (\ldots)\exp(-i\omega\tau)d\tau \propto \begin{cases} t, & \omega = 0, \\ e^{-i\omega t/2}\dfrac{\sin(\omega t/2)}{\omega/2}, & \omega \neq 0. \end{cases} \tag{D.50}$$

If $\omega = 0$, the term grows with time t after the integration, but if $\omega \neq 0$, the term oscillates with t and is inversely proportional to ω. To put it another way, $\exp(-i\omega\tau) = \cos(\omega\tau) - i\sin(\omega\tau)$ consists of a cosine and a sine, which go positive and negative. In an integral over τ, the positive parts would cancel the negative parts, leaving only a small value. If $\omega = 0$, on the other hand, the integral can grow with t.

The argument is admittedly heuristic, but the approximation is very popular and useful. It can sometimes be checked by comparing results from the full model with those obtained using the approximation (although the approximation wouldn't be useful if the full model could be solved.)

D.6. Density operator

Very often we don't know which state a quantum system is in exactly. We may instead have a set of possible states

$$\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_M\rangle\}. \tag{D.51}$$

Suppose also that we know each state $|\psi_m\rangle$ would occur with probability p_m. To model the state of the system *on average*, we use the density operator

$$\boxed{\hat{\rho} = \sum_{m=1}^{M} p_m |\psi_m\rangle\langle\psi_m|.} \tag{D.52}$$

Obviously we must have

$$\sum_{m=1}^{M} p_m = 1, \tag{D.53}$$

so that $\{p_m\}$ is a probability distribution. Note that the number of possible states M here has no relation with the dimension of the Hilbert space (M can be any number from 1 to ∞), and the set of possible states need not be orthogonal, although we still require each possible state $|\psi_m\rangle$ to be normalized, that is,

$$\langle\psi_m|\psi_m\rangle = 1. \tag{D.54}$$

$\hat{\rho}$ is convenient because the expected value of any operator $\hat{A}$ can now be written as

$$\langle A\rangle = \sum_m \langle\psi_m|\,\hat{U}^\dagger(t)\hat{A}\hat{U}(t)\,|\psi_m\rangle\,p_m = \boxed{\operatorname{tr}\Big[\hat{A}\hat{U}(t)\hat{\rho}\hat{U}^\dagger(t)\Big].} \tag{D.55}$$

Instead of evolving each $|\psi_m\rangle$ using $\hat{U}(t)$, we can simply compute the **Schrödinger-picture density operator** using one formula

$$\boxed{\hat{\rho}(t) = \hat{U}(t)\hat{\rho}\hat{U}^\dagger(t).} \tag{D.56}$$

When $p_m = \delta_{ml}$ is a Kronecker delta, the quantum system is definitely in state $|\psi_l\rangle$. Then we say that the state in terms of the density operator $\hat{\rho} = |\psi_l\rangle\langle\psi_l|$ is **pure**; otherwise we say that the state is **mixed**.

More generally, we may assume that the quantum state $|\psi_X\rangle$ depends on a classical random variable X. The density operator is then the expected value of $|\psi_X\rangle\langle\psi_X|$, written as

$$\hat{\rho} = \mathbb{E}\left(|\psi_X\rangle\langle\psi_X|\right). \tag{D.57}$$

For example, if the sample space Ω of the random variable is discrete and the probability mass function of X is $P_X(x)$, then the density operator is written as

$$\hat{\rho} = \sum_{x\in\Omega} P_X(x)\,|\psi_x\rangle\langle\psi_x|\,. \tag{D.58}$$

If the sample space Ω is $\mathbb{R}^n$ and the probability density function is $f_X(\boldsymbol{x})$, then the density operator is written as

$$\hat{\rho} = \int f_X(\boldsymbol{x})\,|\psi_{\boldsymbol{x}}\rangle\langle\psi_{\boldsymbol{x}}|\,d^n\boldsymbol{x}. \tag{D.59}$$

Note that this randomness about the quantum state is not the same as the randomness in a measurement outcome. A state is mixed because of technical imperfections, e.g., it depends on a classical random variable. The randomness due to Born's rule, on the other hand, is fundamental: even if the state is pure, the measurement outcome is random (except in very special cases).

One thing to note is that, given a density operator $\hat{\rho}$, we usually can't tell the set of pure states $\{|\psi_m\rangle\}$ and the probability distribution $\{p_m\}$ that give rise to the $\hat{\rho}$. In other words, there may be another set of pure states $\{|\phi_l\rangle\}$ and another probability distribution $\{p'_l\}$ that give the same $\hat{\rho}$:

$$\hat{\rho} = \sum_m p_m\,|\psi_m\rangle\langle\psi_m| = \sum_l p'_l\,|\phi_l\rangle\langle\phi_l|\,. \tag{D.60}$$

Since $\hat{\rho}$ is a Hermitian and positive-semidefinite operator, we can always write it in the diagonal form

$$\hat{\rho} = \sum_n \lambda_n\,|e_n\rangle\langle e_n|\,, \tag{D.61}$$

where each $|e_n\rangle$ is an eigenvector of $\hat{\rho}$ with eigenvalue λ_n. The eigenvalues, all nonnegative and summing to 1, can be regarded as a probability distribution, but that's just one way of writing $\hat{\rho}$ as a mixture of pure states, there may be many other ways.

Exercise D.9. Prove that $\hat{\rho}$ is Hermitian and positive-semidefinite. Prove that $\operatorname{tr}\hat{\rho} = 1$.

Exercise D.10. If $\hat{\rho}$ is pure, prove that only one of its eigenvalues is nonzero. Find this eigenvalue.

Exercise D.11. Derive the Schrödinger equation for a density operator

$$\frac{d\hat{\rho}(t)}{dt} = -i\Big[\hat{H}, \hat{\rho}(t)\Big]. \tag{D.62}$$

Exercise D.12. Following Exercise D.4, prove that the expected value of a measurement outcome is given by

$$\boxed{\langle A\rangle = \mathrm{tr}\left[\hat{A}\hat{\rho}(t)\right],} \tag{D.63}$$

and the variance is given by

$$\boxed{\left\langle \Delta A^2\right\rangle = \mathrm{tr}\left[\left(\hat{A}-\langle A\rangle\right)^2\hat{\rho}(t)\right] = \mathrm{tr}\left[\hat{A}^2\hat{\rho}(t)\right] - \left\{\mathrm{tr}\left[\hat{A}\hat{\rho}(t)\right]\right\}^2.} \tag{D.64}$$

APPENDIX E

Quantization of EM Fields: Details*

Consider the classical Maxwell equations:

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0}, \qquad \nabla \cdot \boldsymbol{B} = 0, \qquad \frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}, \qquad \frac{\partial \boldsymbol{E}}{\partial t} = c^2 \nabla \times \boldsymbol{B} - \frac{1}{\epsilon_0}\boldsymbol{J}. \tag{E.1}$$

Our goal is to convert these equations to Heisenberg equations of motion in the form of

$$\frac{d\hat{O}(t)}{dt} = -\frac{i}{\hbar}\Big[\hat{O}(t), \hat{H}\Big] \tag{E.2}$$

by converting $\boldsymbol{E}$, $\boldsymbol{B}$, ρ, and $\boldsymbol{J}$ to operators.

E.1. Helmholtz decomposition

The equations will look simpler if we perform the Fourier transform of each field. Define the Fourier transform of a vector field $\boldsymbol{F}(\boldsymbol{r})$ as

$$\boldsymbol{\mathcal{F}}(\boldsymbol{k}) \equiv \frac{1}{(2\pi)^{3/2}} \iiint \boldsymbol{F}(\boldsymbol{r}) \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}) d^3\boldsymbol{r}. \tag{E.3}$$

The inverse Fourier transform is given by

$$\boldsymbol{F}(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} \iiint \boldsymbol{\mathcal{F}}(\boldsymbol{k}) \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) d^3\boldsymbol{k}. \tag{E.4}$$

We use the symbol $\boldsymbol{F}(\boldsymbol{r}) \to \boldsymbol{\mathcal{F}}(\boldsymbol{k})$ to denote the Fourier transform. For a given $\boldsymbol{k}$ in $\boldsymbol{k}$ space, any vector field $\boldsymbol{\mathcal{F}}(\boldsymbol{k})$ is a vector that can be decomposed as

$$\boldsymbol{\mathcal{F}}(\boldsymbol{k}) = \tilde{\boldsymbol{e}}_{\boldsymbol{k},1}\mathcal{F}_1(\boldsymbol{k}) + \tilde{\boldsymbol{e}}_{\boldsymbol{k},2}\mathcal{F}_2(\boldsymbol{k}) + \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}\mathcal{F}_3(\boldsymbol{k}), \qquad \mathcal{F}_s(\boldsymbol{k}) \equiv \tilde{\boldsymbol{e}}^*_{\boldsymbol{k},s} \cdot \boldsymbol{\mathcal{F}}(\boldsymbol{k}), \tag{E.5}$$

in terms of three orthonormal vectors $\tilde{\boldsymbol{e}}_{\boldsymbol{k},1}, \tilde{\boldsymbol{e}}_{\boldsymbol{k},2}, \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}$ that satisfy

$$\tilde{\boldsymbol{e}}^*_{\boldsymbol{k},s} \cdot \tilde{\boldsymbol{e}}_{\boldsymbol{k},s'} = \delta_{ss'}. \tag{E.6}$$

It will be convenient to assume

$$\boxed{\tilde{\boldsymbol{e}}_{\boldsymbol{k},3} = \frac{\boldsymbol{k}}{k},} \qquad k \equiv |\boldsymbol{k}|, \tag{E.7}$$

so the third unit vector $\tilde{\boldsymbol{e}}_{\boldsymbol{k},3}$ is in the direction of the wavevector $\boldsymbol{k}$, while $\tilde{\boldsymbol{e}}_{\boldsymbol{k},1}$ and $\tilde{\boldsymbol{e}}_{\boldsymbol{k},2}$ are unit vectors that are orthogonal to $\boldsymbol{k}$ and to each other. Define

$$\boldsymbol{\mathcal{F}}_{\parallel}(\boldsymbol{k}) \equiv \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}\mathcal{F}_3(\boldsymbol{k}), \tag{E.8}$$

$$\boldsymbol{\mathcal{F}}_{\perp}(\boldsymbol{k}) \equiv \tilde{\boldsymbol{e}}_{\boldsymbol{k},1}\mathcal{F}_1(\boldsymbol{k}) + \tilde{\boldsymbol{e}}_{\boldsymbol{k},2}\mathcal{F}_2(\boldsymbol{k}) = \boldsymbol{\mathcal{F}}(\boldsymbol{k}) - \boldsymbol{\mathcal{F}}_{\parallel}(\boldsymbol{k}). \tag{E.9}$$

In other words, $\boldsymbol{\mathcal{F}}_{\parallel}(\boldsymbol{k})$ is the component of the vector field that is parallel to $\boldsymbol{k}$, while $\boldsymbol{\mathcal{F}}_{\perp}(\boldsymbol{k})$ is the component that is orthogonal to $\boldsymbol{k}$. $\boldsymbol{\mathcal{F}}_{\parallel}$ is called a longitudinal field, $\boldsymbol{\mathcal{F}}_{\perp}$ a transverse field, and

$$\boldsymbol{\mathcal{F}}(\boldsymbol{k}) = \boldsymbol{\mathcal{F}}_{\perp}(\boldsymbol{k}) + \boldsymbol{\mathcal{F}}_{\parallel}(\boldsymbol{k}) \tag{E.10}$$

the Helmholtz decomposition. We can transform these $\boldsymbol{k}$-space vector fields back to the real space to write the decomposition as

$$\boldsymbol{F}(\boldsymbol{r}) = \boldsymbol{F}_{\perp}(\boldsymbol{r}) + \boldsymbol{F}_{\parallel}(\boldsymbol{r}), \tag{E.11}$$

where $\boldsymbol{F}_\perp(\boldsymbol{r})$ and $\boldsymbol{F}_\parallel(\boldsymbol{r})$ are the inverse Fourier transforms of $\boldsymbol{\mathcal{F}}_\perp(\boldsymbol{k})$ and $\boldsymbol{\mathcal{F}}_\parallel(\boldsymbol{k})$, respectively.

$\boldsymbol{F}(\boldsymbol{r})$ is real if and only if

$$\boldsymbol{\mathcal{F}}(\boldsymbol{k}) = \boldsymbol{\mathcal{F}}^*(-\boldsymbol{k}). \tag{E.12}$$

If $\boldsymbol{F}(\boldsymbol{r})$ is real, then $\boldsymbol{F}_\parallel(\boldsymbol{r})$ is also real, since

$$\boldsymbol{\mathcal{F}}_\parallel(\boldsymbol{k}) = \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}\big[\tilde{\boldsymbol{e}}^*_{\boldsymbol{k},3}\cdot\boldsymbol{\mathcal{F}}(\boldsymbol{k})\big] = \frac{\boldsymbol{k}}{|\boldsymbol{k}|}\left[\frac{\boldsymbol{k}}{|\boldsymbol{k}|}\cdot\boldsymbol{\mathcal{F}}(\boldsymbol{k})\right] = \boldsymbol{\mathcal{F}}^*_\parallel(-\boldsymbol{k}). \tag{E.13}$$

It follows that $\boldsymbol{F}_\perp(\boldsymbol{r}) = \boldsymbol{F}(\boldsymbol{r}) - \boldsymbol{F}_\parallel(\boldsymbol{r})$ is also real.

The transverse and longitudinal fields obey the properties

$$\boldsymbol{k}\cdot\boldsymbol{\mathcal{F}}_\perp = 0, \qquad \boldsymbol{k}\times\boldsymbol{\mathcal{F}}_\parallel = 0, \tag{E.14}$$

$$\boldsymbol{k}\cdot\boldsymbol{\mathcal{F}} = \boldsymbol{k}\cdot(\boldsymbol{\mathcal{F}}_\parallel+\boldsymbol{\mathcal{F}}_\perp) = \boldsymbol{k}\cdot\boldsymbol{\mathcal{F}}_\parallel = k\mathcal{F}_3, \qquad \boldsymbol{k}\times\boldsymbol{\mathcal{F}} = \boldsymbol{k}\times(\boldsymbol{\mathcal{F}}_\parallel+\boldsymbol{\mathcal{F}}_\perp) = \boldsymbol{k}\times\boldsymbol{\mathcal{F}}_\perp. \tag{E.15}$$

In particular, $\boldsymbol{k}\times\boldsymbol{\mathcal{F}} = \boldsymbol{k}\times\boldsymbol{\mathcal{F}}_\perp$ is orthogonal to $\boldsymbol{k}$.

Given another vector field $\boldsymbol{\mathcal{G}}(\boldsymbol{k}) = \boldsymbol{\mathcal{G}}_\perp(\boldsymbol{k}) + \boldsymbol{\mathcal{G}}_\parallel(\boldsymbol{k})$, we have

$$\boldsymbol{\mathcal{F}}^*_\perp\cdot\boldsymbol{\mathcal{G}}_\parallel = 0, \qquad \boldsymbol{\mathcal{F}}^*\cdot\boldsymbol{\mathcal{G}} = \boldsymbol{\mathcal{F}}^*_\perp\cdot\boldsymbol{\mathcal{G}}_\perp + \boldsymbol{\mathcal{F}}^*_\parallel\cdot\boldsymbol{\mathcal{G}}_\parallel, \tag{E.16}$$

and Parseval's theorem gives

$$\iiint \boldsymbol{F}^*(\boldsymbol{r})\cdot\boldsymbol{G}(\boldsymbol{r})d^3\boldsymbol{r} = \iiint \boldsymbol{\mathcal{F}}^*(\boldsymbol{k})\cdot\boldsymbol{\mathcal{G}}(\boldsymbol{k})d^3\boldsymbol{k}. \tag{E.17}$$

E.2. Maxwell's equations with Helmholtz decomposition

Let

$$\boldsymbol{E}(\boldsymbol{r},t)\to\boldsymbol{\mathcal{E}}(\boldsymbol{k},t), \qquad \boldsymbol{B}(\boldsymbol{r},t)\to\boldsymbol{\mathcal{B}}(\boldsymbol{k},t), \qquad \rho(\boldsymbol{r},t)\to\varrho(\boldsymbol{k},t), \qquad \boldsymbol{J}(\boldsymbol{r},t)\to\boldsymbol{\mathcal{J}}(\boldsymbol{k},t). \tag{E.18}$$

Maxwell's equations in $\boldsymbol{k}$ space become

$$i\boldsymbol{k}\cdot\boldsymbol{\mathcal{E}} = \frac{\varrho}{\epsilon_0}, \qquad i\boldsymbol{k}\cdot\boldsymbol{\mathcal{B}} = 0, \qquad \frac{\partial\boldsymbol{\mathcal{B}}}{\partial t} = -i\boldsymbol{k}\times\boldsymbol{\mathcal{E}}, \qquad \frac{\partial\boldsymbol{\mathcal{E}}}{\partial t} = ic^2\boldsymbol{k}\times\boldsymbol{\mathcal{B}} - \frac{1}{\epsilon_0}\boldsymbol{\mathcal{J}}. \tag{E.19}$$

Applying the Helmholtz decomposition to all the fields, the equations become

$$i\boldsymbol{k}\cdot\boldsymbol{\mathcal{E}}_\parallel = ik\mathcal{E}_3 = \frac{\varrho}{\epsilon_0}, \qquad i\boldsymbol{k}\cdot\boldsymbol{\mathcal{B}} = ik\mathcal{B}_3 = 0, \tag{E.20}$$

$$\frac{\partial\boldsymbol{\mathcal{B}}_\perp}{\partial t} = -i\boldsymbol{k}\times\boldsymbol{\mathcal{E}}_\perp, \qquad \frac{\partial\boldsymbol{\mathcal{E}}_\perp}{\partial t} = ic^2\boldsymbol{k}\times\boldsymbol{\mathcal{B}}_\perp - \frac{1}{\epsilon_0}\boldsymbol{\mathcal{J}}_\perp, \tag{E.21}$$

$$\frac{\partial\boldsymbol{\mathcal{E}}_\parallel}{\partial t} = -\frac{1}{\epsilon_0}\boldsymbol{\mathcal{J}}_\parallel. \tag{E.22}$$

Notice the following:

(1) We will ignore the $\boldsymbol{k}=0$ case and assume $\boldsymbol{k}\neq 0$ and thus $k\neq 0$.

(2) Gauss's law for magnetism implies that $B_3 = 0$, $\boldsymbol{\mathcal{B}}_\parallel = \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}B_3 = 0$, so the magnetic field only has the transverse component

$$\boxed{\boldsymbol{\mathcal{B}} = \boldsymbol{\mathcal{B}}_\perp.} \tag{E.23}$$

(3) The longitudinal component $\boldsymbol{\mathcal{E}}_\parallel = \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}\mathcal{E}_3$ of the electric field is determined by the charge density through the equation

$$\boxed{\mathcal{E}_3(\boldsymbol{k},t) = \frac{\varrho(\boldsymbol{k},t)}{ik\epsilon_0},} \tag{E.24}$$

which shows that $\mathcal{E}_3(\boldsymbol{k},t)$ is **not a separate degree of freedom**, because its value is slaved at all times to $\varrho(\boldsymbol{k},t)$ that is determined by the matter. Contrast Eq. (E.24) with a differential equation $\partial O(t)/\partial t = \ldots$,

which allows an arbitrary initial condition $O(t=0)$ for the variable. In particular, if $\varrho(\boldsymbol{k},t)=0$, then $\mathcal{E}_3=0$, and the longitudinal electric field cannot survive without a charge density.

(4) Eq. (E.24) already tells us $\mathcal{E}_3(\boldsymbol{k},t)$, so Eq. (E.22) seems a bit redundant. To see the physical meaning of Eq. (E.22), combine it with Eq. (E.24) to write an equation in terms of matter variables ϱ and $\boldsymbol{\mathcal{J}}$ only:

$$\frac{\partial \mathcal{E}_3}{\partial t}=\frac{1}{ik\epsilon_0}\frac{\partial \varrho}{\partial t}=-\frac{1}{\epsilon_0}\mathcal{J}_3, \qquad \frac{\partial \varrho}{\partial t}+ik\mathcal{J}_3=0, \qquad \frac{\partial \varrho}{\partial t}+i\boldsymbol{k}\cdot\boldsymbol{\mathcal{J}}=0. \tag{E.25}$$

This is simply the $\boldsymbol{k}$-space version of the charge continuity equation

$$\frac{\partial \rho}{\partial t}+\nabla\cdot\boldsymbol{J}=0, \tag{E.26}$$

so Eq. (E.22) is in fact a statement about charge conservation.

E.3. Normal variables for transverse fields

Only the transverse components of the EM fields $\boldsymbol{\mathcal{E}}_\perp$ and $\boldsymbol{\mathcal{B}}_\perp$ can survive when there is no source, so they are also called free fields. Their equations of motion are given by

$$\boxed{\frac{\partial \boldsymbol{\mathcal{B}}_\perp}{\partial t}=-i\boldsymbol{k}\times\boldsymbol{\mathcal{E}}_\perp,} \qquad \boxed{\frac{\partial \boldsymbol{\mathcal{E}}_\perp}{\partial t}=ic^2\boldsymbol{k}\times\boldsymbol{\mathcal{B}}_\perp-\frac{1}{\epsilon_0}\boldsymbol{\mathcal{J}}_\perp.} \tag{E.27}$$

To make them look more like Heisenberg equations of motion, we introduce the scalar potential $\phi(\boldsymbol{r},t)$ and the vector potential $\boldsymbol{A}(\boldsymbol{r},t)$, which obey

$$\boldsymbol{E}=-\nabla\phi-\frac{\partial \boldsymbol{A}}{\partial t}, \qquad \boldsymbol{B}=\nabla\times\boldsymbol{A}. \tag{E.28}$$

Going to the $\boldsymbol{k}$ space with

$$\phi(\boldsymbol{r},t)\to\varphi(\boldsymbol{k},t), \qquad \boldsymbol{A}(\boldsymbol{r},t)\to\boldsymbol{\mathcal{A}}(\boldsymbol{k},t), \tag{E.29}$$

and decomposing the vector potential as $\boldsymbol{\mathcal{A}}=\boldsymbol{\mathcal{A}}_\parallel+\boldsymbol{\mathcal{A}}_\perp$, we obtain

$$\boldsymbol{\mathcal{E}}_\parallel=-i\boldsymbol{k}\varphi-\frac{\partial \boldsymbol{\mathcal{A}}_\parallel}{\partial t}, \qquad \boldsymbol{\mathcal{E}}_\perp=-\frac{\partial \boldsymbol{\mathcal{A}}_\perp}{\partial t}, \qquad \boldsymbol{\mathcal{B}}=\boldsymbol{\mathcal{B}}_\perp=i\boldsymbol{k}\times\boldsymbol{\mathcal{A}}_\perp. \tag{E.30}$$

Eqs. (E.27) are then equivalent to

$$\frac{\partial \boldsymbol{\mathcal{A}}_\perp}{\partial t}=-\boldsymbol{\mathcal{E}}_\perp, \qquad -\frac{\partial \boldsymbol{\mathcal{E}}_\perp}{\partial t}=-c^2k^2\boldsymbol{\mathcal{A}}_\perp+\frac{1}{\epsilon_0}\boldsymbol{\mathcal{J}}_\perp. \tag{E.31}$$

Recall that each transverse component $\boldsymbol{\mathcal{F}}_\perp=\mathcal{F}_1\tilde{\boldsymbol{e}}_{\boldsymbol{k},1}+\mathcal{F}_2\tilde{\boldsymbol{e}}_{\boldsymbol{k},2}$ of a vector field has two components in two directions. Eqs. (E.31) can then be rewritten as

$$\frac{\partial \mathcal{A}_s}{\partial t}=-\mathcal{E}_s, \qquad -\frac{\partial \mathcal{E}_s}{\partial t}=-c^2k^2\mathcal{A}_s+\frac{1}{\epsilon_0}\mathcal{J}_s, \qquad s=1,2. \tag{E.32}$$

For each $j\equiv(\boldsymbol{k},s)$, $\mathcal{A}_s(\boldsymbol{k},t)$ behaves like a position variable of a harmonic oscillator, $-\mathcal{E}_s(\boldsymbol{k},t)$ behaves like a momentum variable, and $\mathcal{J}_s(\boldsymbol{k},t)$ behaves like a force, except that they are all complex. Despite the complexity, we can turn them into an equation of motion for a harmonic oscillator by defining a complex **normal variable**

$$\boxed{\alpha_s(\boldsymbol{k},t)\equiv C\Big[\omega^{1/2}\mathcal{A}_s(\boldsymbol{k},t)-i\omega^{-1/2}\mathcal{E}_s(\boldsymbol{k},t)\Big],} \qquad \boxed{\omega\equiv ck,} \tag{E.33}$$

where C is a real constant, so that

$$\boxed{\frac{\partial \alpha_s}{\partial t}=-i\omega\alpha_s+\frac{iC}{\epsilon_0\sqrt{\omega}}\mathcal{J}_s,} \qquad \boxed{s=1,2.} \tag{E.34}$$

This differential equation shows that each mode labeled by $(\boldsymbol{k},s)$ is a separate **degree of freedom**—free in the sense that it allows an arbitrary initial condition $\alpha_s(\boldsymbol{k},0)$ for each $(\boldsymbol{k},s)$.

The normal variables fully model the dynamics of the transverse fields, since we can write $\boldsymbol{\mathcal{A}}_\perp$ and $\boldsymbol{\mathcal{E}}_\perp$ as functions of the normal variables. To do so, recall that, since $\boldsymbol{A}$ and $\boldsymbol{E}$ in real space are real, $\boldsymbol{\mathcal{A}}_\perp$ and $\boldsymbol{\mathcal{E}}_\perp$ obey the property

$$\boldsymbol{\mathcal{A}}_\perp(\boldsymbol{k},t)=\boldsymbol{\mathcal{A}}_\perp^*(-\boldsymbol{k},t)=\sum_s \mathcal{A}_s^*(-\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*,\qquad \boldsymbol{\mathcal{E}}_\perp(\boldsymbol{k},t)=\boldsymbol{\mathcal{E}}_\perp^*(-\boldsymbol{k},t)=\sum_s \mathcal{E}_s^*(-\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*. \tag{E.35}$$

Now consider

$$\sum_s \alpha_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}=C\Big[\omega^{1/2}\boldsymbol{\mathcal{A}}_\perp(\boldsymbol{k},t)-i\omega^{-1/2}\boldsymbol{\mathcal{E}}_\perp(\boldsymbol{k},t)\Big], \tag{E.36}$$

$$\sum_s \alpha_s^*(-\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*=C\Big[\omega^{1/2}\boldsymbol{\mathcal{A}}_\perp^*(-\boldsymbol{k},t)+i\omega^{-1/2}\boldsymbol{\mathcal{E}}_\perp^*(-\boldsymbol{k},t)\Big]=C\Big[\omega^{1/2}\boldsymbol{\mathcal{A}}_\perp(\boldsymbol{k},t)+i\omega^{-1/2}\boldsymbol{\mathcal{E}}_\perp(\boldsymbol{k},t)\Big]. \tag{E.37}$$

The two equations can be combined to give

$$\boldsymbol{\mathcal{A}}_\perp(\boldsymbol{k},t)=\frac{1}{2C\omega^{1/2}}\sum_s\big[\alpha_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}+\alpha_s^*(-\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*\big], \tag{E.38}$$

$$\boldsymbol{\mathcal{E}}_\perp(\boldsymbol{k},t)=\frac{\omega^{1/2}}{2C}\sum_s\big[i\alpha_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}-i\alpha_s^*(-\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*\big]. \tag{E.39}$$

These fields can be transformed back to real space to give

$$\boxed{\boldsymbol{A}_\perp(\boldsymbol{r},t)=\frac{1}{(2\pi)^{3/2}2C}\sum_{s=1}^{2}\iiint \omega^{-1/2}[\alpha_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})+\text{c.c.}]d^3\boldsymbol{k},} \tag{E.40}$$

$$\boxed{\boldsymbol{E}_\perp(\boldsymbol{r},t)=\frac{1}{(2\pi)^{3/2}2C}\sum_{s=1}^{2}\iiint \omega^{1/2}[i\alpha_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})+\text{c.c.}]d^3\boldsymbol{k}.} \tag{E.41}$$

These expressions are consistent with the classical model in Chapter 2 if we take the $L\to\infty$ limit.

E.4. Gauge invariance of $\boldsymbol{\mathcal{A}}_\perp$

Recall that, given any scalar field $\gamma(\boldsymbol{r},t)$, a gauge change given by

$$\phi'=\phi-\frac{\partial\gamma}{\partial t},\qquad\qquad \boldsymbol{A}'=\boldsymbol{A}+\nabla\gamma \tag{E.42}$$

has no effect on the $\boldsymbol{E}$ and $\boldsymbol{B}$ fields:

$$\boldsymbol{E}=-\nabla\phi'-\frac{\partial\boldsymbol{A}'}{\partial t},\qquad\qquad \boldsymbol{B}=\nabla\times\boldsymbol{A}'. \tag{E.43}$$

In $\boldsymbol{k}$ space, let $\gamma(\boldsymbol{r},t)\to\Gamma(\boldsymbol{k},t)$. Since $\nabla\gamma\to i\boldsymbol{k}\Gamma$, which is parallel to $\boldsymbol{k}$, any gauge change has no effect on the transverse component $\boldsymbol{\mathcal{A}}_\perp$:

$$\varphi'=\varphi-\frac{\partial\Gamma}{\partial t},\qquad\qquad \boldsymbol{\mathcal{A}}_\parallel'=\boldsymbol{\mathcal{A}}_\parallel+i\boldsymbol{k}\Gamma,\qquad\qquad \boxed{\boldsymbol{\mathcal{A}}_\perp'=\boldsymbol{\mathcal{A}}_\perp.} \tag{E.44}$$

Hence, there is no need to worry about gauge ambiguity when we deal with $\boldsymbol{\mathcal{A}}_\perp$; it is unique given $\boldsymbol{E}$ and $\boldsymbol{B}$.

E.5. Canonical quantization of the transverse fields

Consider a fixed time $t = 0$. The total EM energy is given by

$$H = \frac{1}{2}\iiint \left(\epsilon_0 \boldsymbol{E}\cdot\boldsymbol{E} + \frac{1}{\mu_0}\boldsymbol{B}\cdot\boldsymbol{B}\right) d^3\boldsymbol{r} \tag{E.45}$$

$$= \frac{1}{2}\iiint \left(\epsilon_0 \boldsymbol{\mathcal{E}}^*\cdot\boldsymbol{\mathcal{E}} + \frac{1}{\mu_0}\boldsymbol{\mathcal{B}}^*\cdot\boldsymbol{\mathcal{B}}\right) d^3\boldsymbol{k} \qquad \text{(Parseval)} \tag{E.46}$$

$$= \frac{1}{2}\iiint \left(\epsilon_0 \boldsymbol{\mathcal{E}}_\parallel^*\cdot\boldsymbol{\mathcal{E}}_\parallel + \epsilon_0 \boldsymbol{\mathcal{E}}_\perp^*\cdot\boldsymbol{\mathcal{E}}_\perp + \frac{1}{\mu_0}\boldsymbol{\mathcal{B}}_\perp^*\cdot\boldsymbol{\mathcal{B}}_\perp\right) d^3\boldsymbol{k} \qquad \text{(Helmholtz)} \tag{E.47}$$

$$= \frac{\epsilon_0}{2}\iiint \left(\boldsymbol{\mathcal{E}}_\parallel^*\cdot\boldsymbol{\mathcal{E}}_\parallel + \boldsymbol{\mathcal{E}}_\perp^*\cdot\boldsymbol{\mathcal{E}}_\perp + c^2k^2\boldsymbol{\mathcal{A}}_\perp^*\cdot\boldsymbol{\mathcal{A}}_\perp\right) d^3\boldsymbol{k}. \qquad (\boldsymbol{\mathcal{B}}_\perp = i\boldsymbol{k}\times\boldsymbol{\mathcal{A}}_\perp, \boldsymbol{\mathcal{A}}_\perp \perp \boldsymbol{k}) \tag{E.48}$$

Define

$$H = H_\parallel + H_\perp, \tag{E.49}$$

$$H_\parallel \equiv \frac{\epsilon_0}{2}\iiint \boldsymbol{\mathcal{E}}_\parallel^*\cdot\boldsymbol{\mathcal{E}}_\parallel d^3\boldsymbol{k}, \tag{E.50}$$

$$H_\perp \equiv \frac{\epsilon_0}{2}\iiint \left(\boldsymbol{\mathcal{E}}_\perp^*\cdot\boldsymbol{\mathcal{E}}_\perp + c^2k^2\boldsymbol{\mathcal{A}}_\perp^*\cdot\boldsymbol{\mathcal{A}}_\perp\right) d^3\boldsymbol{k} = \iiint \frac{\epsilon_0\omega}{2C^2}\sum_{s=1}^{2}|\alpha_s(\boldsymbol{k})|^2 d^3\boldsymbol{k}, \tag{E.51}$$

where $H_\perp$ is the energy of the free transverse fields. We defer the quantization of $H_\parallel$ in terms of $\boldsymbol{\mathcal{E}}_\parallel$ to Sec. E.6 later and quantize the transverse EM fields here by setting

$$\frac{\epsilon_0\omega}{2C^2} = \hbar\omega, \qquad\qquad C = \sqrt{\frac{\epsilon_0}{2\hbar}} \tag{E.52}$$

and replacing $\alpha_s(\boldsymbol{k})$ with $\hat{a}_s(\boldsymbol{k})$ on some Hilbert space $\mathcal{H}_\perp$. Assume the commutation relation

$$\boxed{\left[\hat{a}_s(\boldsymbol{k}), \hat{a}_{s'}^\dagger(\boldsymbol{k}')\right] = \delta_{ss'}\delta^3(\boldsymbol{k}-\boldsymbol{k}').} \tag{E.53}$$

Then

$$\boxed{\hat{H}_\perp = \iiint \hbar\omega\sum_{s=1}^{2}\hat{a}_s^\dagger(\boldsymbol{k})\hat{a}_s(\boldsymbol{k})d^3\boldsymbol{k},} \tag{E.54}$$

and the operators for the transverse vector potential and the transverse electric field at $t = 0$ can be defined as

$$\hat{\boldsymbol{\mathcal{A}}}_\perp(\boldsymbol{k}) \equiv \sqrt{\frac{\hbar}{2\epsilon_0\omega}}\sum_{s=1}^{2}\left[\hat{a}_s(\boldsymbol{k})\tilde{\boldsymbol{e}}_{\boldsymbol{k},s} + \hat{a}_s^\dagger(-\boldsymbol{k})\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*\right], \tag{E.55}$$

$$\hat{\boldsymbol{\mathcal{E}}}_\perp(\boldsymbol{k}) \equiv \sqrt{\frac{\hbar\omega}{2\epsilon_0}}\sum_{s=1}^{2}\left[i\hat{a}_s(\boldsymbol{k})\tilde{\boldsymbol{e}}_{\boldsymbol{k},s} - i\hat{a}_s^\dagger(-\boldsymbol{k})\tilde{\boldsymbol{e}}_{-\boldsymbol{k},s}^*\right], \tag{E.56}$$

which are consistent with Eqs. (E.38) and (E.39) at $t = 0$. The Heisenberg equations of motion for $\hat{\boldsymbol{\mathcal{A}}}_\perp(\boldsymbol{k}, t)$ and $\hat{\boldsymbol{\mathcal{E}}}_\perp(\boldsymbol{k}, t)$ can be derived from

$$\boxed{\hat{a}_s(\boldsymbol{k}, t) = \hat{a}_s(\boldsymbol{k})\exp(-i\omega t).} \tag{E.57}$$

In real space,

$$\hat{\boldsymbol{A}}_\perp(\boldsymbol{r},t) \equiv \frac{1}{(2\pi)^{3/2}} \iiint \hat{\boldsymbol{\mathcal{A}}}_\perp(\boldsymbol{k},t)\exp(i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{k} \tag{E.58}$$

$$= \boxed{\frac{1}{(2\pi)^{3/2}} \sum_{s=1}^{2} \iiint \sqrt{\frac{\hbar}{2\epsilon_0\omega}} \Big[\hat{a}_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \text{H.c.}\Big] d^3\boldsymbol{k},} \tag{E.59}$$

$$\hat{\boldsymbol{E}}_\perp(\boldsymbol{r},t) \equiv \frac{1}{(2\pi)^{3/2}} \iiint \hat{\boldsymbol{\mathcal{E}}}_\perp(\boldsymbol{k},t)\exp(i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{k} \tag{E.60}$$

$$= \boxed{\frac{1}{(2\pi)^{3/2}} \sum_{s=1}^{2} \iiint \sqrt{\frac{\hbar\omega}{2\epsilon_0}} \Big[i\hat{a}_s(\boldsymbol{k},t)\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \text{H.c.}\Big] d^3\boldsymbol{k},} \tag{E.61}$$

which are consistent with Eqs. (E.40) and (E.41) as well as the classical and quantum models in Chapters 2 and 3 for free EM fields, where $\hat{H}_{\text{EM}} = \hat{H}_\perp$ is assumed.

E.6. Quantization of the longitudinal electric field

The quantization of $H_\parallel$ in terms of the longitudinal $\boldsymbol{\mathcal{E}}_\parallel = \tilde{\boldsymbol{e}}_{\boldsymbol{k},3}\mathcal{E}_3$ is quite different. When there is no matter, $\mathcal{E}_3 = 0$, and there is no need to quantize it. When there is matter, we should introduce a new Hilbert space $\mathcal{H}_{\text{matter}}$ and additional terms to the Hamiltonian that model the matter dynamics and the light-matter interaction. In that case, the simplest way of quantizing $\mathcal{E}_3$ is to follow Eq. (E.24) and assume that the longitudinal component at $t = 0$ is equal to

$$\hat{\mathcal{E}}_3(\boldsymbol{k}) = \frac{\hat{\varrho}(\boldsymbol{k})}{ik\epsilon_0}, \tag{E.62}$$

where $\hat{\varrho}(\boldsymbol{k})$ is the charge-density operator on $\mathcal{H}_{\text{matter}}$. The Heisenberg picture

$$\hat{\mathcal{E}}_3(\boldsymbol{k},t) = \frac{\hat{\varrho}(\boldsymbol{k},t)}{ik\epsilon_0} \tag{E.63}$$

is then consistent with the classical Eq. (E.24). This model means that we do not need to introduce any new degree of freedom for the longitudinal electric field, and it suffices to stick to the Hilbert spaces $\mathcal{H}_\perp$ for the transverse fields and $\mathcal{H}_{\text{matter}}$ for the matter. $\hat{\mathcal{E}}_3(\boldsymbol{k})$ is an operator on $\mathcal{H}_{\text{matter}}$, and the quantized $\hat{H}_\parallel$ is also an operator on $\mathcal{H}_{\text{matter}}$:

$$\hat{H}_\parallel = \frac{\epsilon_0}{2} \iiint \hat{\mathcal{E}}_3^\dagger(\boldsymbol{k})\hat{\mathcal{E}}_3(\boldsymbol{k})d^3\boldsymbol{k} = \frac{1}{2\epsilon_0} \iiint \frac{1}{k^2}\hat{\varrho}^\dagger(\boldsymbol{k})\hat{\varrho}(\boldsymbol{k})d^3\boldsymbol{k}. \tag{E.64}$$

E.7. Current source

Let $\hat{H}_{\text{matter}}$ be the matter Hamiltonian on a matter Hilbert space $\mathcal{H}_{\text{matter}}$ and let the interaction Hamiltonian be

$$\hat{\eta} = -\iiint \hat{\boldsymbol{A}}_\perp(\boldsymbol{r})\cdot\hat{\boldsymbol{J}}(\boldsymbol{r})d^3\boldsymbol{r} = -\iiint \hat{\boldsymbol{\mathcal{A}}}_\perp^\dagger(\boldsymbol{k})\cdot\hat{\boldsymbol{\mathcal{J}}}(\boldsymbol{k})d^3\boldsymbol{k}, \tag{E.65}$$

where $\hat{\boldsymbol{J}}(\boldsymbol{r})$ is a current-density operator on $\mathcal{H}_{\text{matter}}$. $\hat{H}_\parallel$ is assumed to be part of $\hat{H}_{\text{matter}}$. The Heisenberg equation of motion for $\hat{a}_s(\boldsymbol{k},t)$ under the Hamiltonian $\hat{H}_{\text{matter}} + \hat{H}_\perp + \hat{\eta}$ becomes

$$\frac{d\hat{a}_s(\boldsymbol{k},t)}{dt} = -i\omega\hat{a}_s(\boldsymbol{k},t) + i\frac{1}{\sqrt{2\epsilon_0\hbar\omega}}\hat{\mathcal{J}}_s(\boldsymbol{k},t), \tag{E.66}$$

which is consistent with the classical Eq. (E.34).

To model the current as classical, as discussed in Sec. 5.2, we go to the interaction picture with $\hat{H}_{\text{easy}} = \hat{H}_{\text{matter}} + \hat{H}_\perp$, leading to

$$\hat{\eta}_{\text{easy}}(t) = -\iiint \hat{\boldsymbol{A}}_\perp(\boldsymbol{r},t)\cdot\hat{\boldsymbol{J}}(\boldsymbol{r},t)d^3\boldsymbol{r}. \tag{E.67}$$

Then we approximate $\hat{\boldsymbol{J}}(\boldsymbol{r},t)$ by a c-number function $\boldsymbol{J}(\boldsymbol{r},t)$.

Do note that the model here is just one possible model of light-matter interaction. Although it serves our purpose in this book, there are many other models that differ in nontrivial ways [42]. For example, when light is coupled to atoms or charged particles in the nonrelativistic limit, the interaction Hamiltonian is a bit more complicated.

E.8. Coulomb gauge

So far we have completely avoided the quantization of φ and $\boldsymbol{\mathcal{A}}_\parallel$, which may appear in the classical Hamiltonian when there is matter. The simplest way is to assume the Coulomb gauge

$$\nabla\cdot\boldsymbol{A}=0, \tag{E.68}$$

which is equivalent to

$$\boldsymbol{\mathcal{A}}_\parallel=0, \qquad\qquad \boldsymbol{\mathcal{A}}=\boldsymbol{\mathcal{A}}_\perp. \tag{E.69}$$

The longitudinal electric field becomes

$$\boldsymbol{\mathcal{E}}_\parallel=-i\boldsymbol{k}\varphi, \qquad\qquad \mathcal{E}_3=-ik\varphi, \qquad\qquad \varphi=-\frac{1}{ik}\mathcal{E}_3=\frac{\varrho}{k^2\epsilon_0}. \tag{E.70}$$

Then there is no need to quantize $\boldsymbol{\mathcal{A}}_\parallel$ and we just treat $\hat{\varphi}$ as a function of $\hat{\varrho}$ if needed (i.e., $\hat{\varphi}(\boldsymbol{k})=\hat{\varrho}(\boldsymbol{k})/(k^2\epsilon_0)$ is an operator on $\mathcal{H}_{\text{matter}}$). The quantized vector potential becomes

$$\boxed{\hat{\boldsymbol{A}}(\boldsymbol{r},t)=\hat{\boldsymbol{A}}_\perp(\boldsymbol{r},t),} \tag{E.71}$$

meaning that we can omit the $\perp$.

The gauge issue is both deep and fundamental in quantum field theory, although it is outside the scope of this book to discuss it. It suffices to point out that the "canonical" Coulomb-gauge treatment here turns out to be equivalent to other treatments that assume other gauges and fully compatible with special relativity [42], even though the quantum formalism treats time differently and its Lorentz invariance is not obvious.

APPENDIX F

EM Fields in Matter*

Matter responds to EM fields by creating a bound charge density $\rho_b(\boldsymbol{r}, t)$ and a bound current density $\boldsymbol{J}_b(\boldsymbol{r}, t)$. We model the effect of the bound charges on the EM fields by assuming a **polarization field** $\boldsymbol{P}(\boldsymbol{r}, t)$ that obeys

$$\nabla \cdot \boldsymbol{P} = -\rho_b, \qquad \frac{\partial \boldsymbol{P}}{\partial t} = \boldsymbol{J}_b. \tag{F.1}$$

Magnetization is negligible at optical frequencies. With these assumptions, $(\rho_b, \boldsymbol{J}_b)$ obey the continuity equation

$$\frac{\partial \rho_b}{\partial t} + \nabla \cdot \boldsymbol{J}_b = 0, \tag{F.2}$$

as expected. Assuming that there is no extra charge or current other than the bound quantities, Gauss' law becomes

$$\nabla \cdot \boldsymbol{E} = \frac{\rho_b}{\epsilon_0} = -\frac{1}{\epsilon_0} \nabla \cdot \boldsymbol{P}, \qquad \nabla \cdot \boldsymbol{D} = 0, \tag{F.3}$$

where

$$\boldsymbol{D} \equiv \epsilon_0 \boldsymbol{E} + \boldsymbol{P} \tag{F.4}$$

is called the displacement field. The modified Ampere's law becomes

$$\nabla \times \boldsymbol{B} = \mu_0 \boldsymbol{J}_b + \mu_0 \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} = \mu_0 \frac{\partial \boldsymbol{P}}{\partial t} + \mu_0 \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} = \mu_0 \frac{\partial \boldsymbol{D}}{\partial t}. \tag{F.5}$$

Remark F.1. *Do not confuse the polarization field with the polarization of a wave; they are completely different things. Unfortunately both terms are standard.*

We can study how the electric field responds to a given $\boldsymbol{P}$ by looking at the equation

$$-\nabla \times (\nabla \times \boldsymbol{E}) - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \mu_0 \frac{\partial^2 \boldsymbol{P}}{\partial t^2}. \tag{F.6}$$

To fully solve for the EM fields, we also need a model of how $\boldsymbol{P}$ responds to the EM fields by studying the dynamics of the matter.

A material is called **dielectric** when $\boldsymbol{P}$ is a function of $\boldsymbol{E}$ only. The simplest model is

$$\boldsymbol{P}(\boldsymbol{r}, t) = \epsilon_0 \chi^{(1)} \boldsymbol{E}(\boldsymbol{r}, t), \tag{F.7}$$

so the polarization field is assumed to respond instantly and locally to the electric field, that is, $\boldsymbol{P}(\boldsymbol{r}, t)$ at each position $\boldsymbol{r}$ and time t depends only on the electric field at that particular position and time. Moreover, $\boldsymbol{P}$ here is assumed to be linear with respect to $\boldsymbol{E}$, and we call this a **linear dielectric** model. As a result of Eq. (F.7), $\boldsymbol{D} = \epsilon_0(1 + \chi^{(1)})\boldsymbol{E}$, $\nabla \cdot \boldsymbol{E} = 0$, and we arrive at the wave equation

$$\nabla^2 \boldsymbol{E} - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \frac{\chi^{(1)}}{c^2} \frac{\partial \boldsymbol{E}}{\partial t}. \tag{F.8}$$

This is a wave equation with speed c/n if we assume the refractive index

$$n = \sqrt{1 + \chi^{(1)}}. \tag{F.9}$$

The net effect is that the wave travels at a different speed c/n in a dielectric, but it is important to keep in mind the underlying mechanism: the EM fields interact with the matter through the polarization field, and the matter is an important participant of the wave dynamics.

To model loss, we assume that the matter consists of damped oscillators. The easiest way is to change Eq. (F.7) to

$$\boldsymbol{P}(\boldsymbol{r},t) = \epsilon_0 \int_{-\infty}^{\infty} \chi^{(1)}(t-t')\boldsymbol{E}(\boldsymbol{r},t')dt', \tag{F.10}$$

where $\chi^{(1)}$ is a Green's function (also called an impulse-response function) that relates the electric field to the polarization field. Causality implies that

$$\chi^{(1)}(t-t') = 0, \quad t' > t, \tag{F.11}$$

so that $\boldsymbol{P}(\boldsymbol{r},t)$ depends only on the past values of the electric field $\{\boldsymbol{E}(\boldsymbol{r},t') : t' \leq t\}$ before time t. It's easier to study this relation in the frequency domain

$$\tilde{\boldsymbol{P}}(\boldsymbol{r},\omega) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \boldsymbol{P}(\boldsymbol{r},t)e^{i\omega t}dt = \epsilon_0 \tilde{\chi}^{(1)}(\omega)\tilde{\boldsymbol{E}}(\boldsymbol{r},\omega), \tag{F.12}$$

and then study $\tilde{\chi}^{(1)}(\omega)$ only within the frequency range of interest. A nonzero imaginary part of $\tilde{\chi}^{(1)}(\omega)$ would correspond to loss or gain. The easiest way to see this is to consider the average power per unit volume lost by the EM field to the matter for a sinusoidal plane wave (the overline denotes averaging over a long time):

$$\frac{\overline{\text{Power}}}{\text{Volume}} = \overline{\boldsymbol{J}_b \cdot \boldsymbol{E}} = \overline{\frac{\partial \boldsymbol{P}}{\partial t} \cdot \boldsymbol{E}} \propto \overline{\left[(-i\omega)\tilde{\chi}^{(1)}(\omega)\alpha e^{-i\omega t} + \text{c.c.}\right](\alpha e^{-i\omega t} + \text{c.c.})} \tag{F.13}$$

$$= -i\omega\tilde{\chi}^{(1)}(\omega)|\alpha|^2 + \text{c.c.} \propto \operatorname{Im}\tilde{\chi}^{(1)}(\omega). \tag{F.14}$$

APPENDIX G

Open Quantum Systems*

An open system refers to a system that interacts with an environment. The hope of open system theory is that, since we care more about the system and less about the environment, our model can be simplified if we study only the effect of the environment on the system of interest.

The subject is huge and this chapter provides only a quick summary; more specialized textbooks, such as Refs. [43, 21, 19, 44, 45, 46, 47], should be consulted for details.

We stick to the Schrödinger picture in this chapter. It is not impossible to use the Heisenberg picture for open quantum systems [48] but the Schrödinger picture is much more popular.

G.1. Density operator

We have introduced the density operator earlier in Sec. D.6 in terms of an average quantum state. Another way of arriving at a density operator is to consider a larger Hilbert space $\mathcal{H} \otimes \mathcal{H}_B$, where $\mathcal{H}$ models the degrees of freedom of a system and $\mathcal{H}_B$ models those of the environment. The environment is also called a bath, a reservoir, or an ancilla (fancy word for an aid), depending on the context. Assume that the system and the environment are in a pure state $|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H}_B$ in the larger Hilbert space, normalized as $\langle\Psi|\Psi\rangle = 1$. Then the expectation of any system observable $\hat{A} \otimes \hat{I}$ becomes

$$\operatorname{tr}\left[\left(\hat{A} \otimes \hat{I}\right) |\Psi\rangle \langle\Psi|\right] = \operatorname{tr}\left[\hat{A} \operatorname{tr}_B \left(|\Psi\rangle \langle\Psi|\right)\right] = \operatorname{tr}\left(\hat{A}\hat{\rho}\right), \tag{G.1}$$

where tr_B is the partial trace with respect to $\mathcal{H}_B$ and

$$\hat{\rho} \equiv \operatorname{tr}_B \left(|\Psi\rangle \langle\Psi|\right) \tag{G.2}$$

is the density operator on the system Hilbert space $\mathcal{H}$. In other words, with the density operator, the expectation with respect to any system observable $\hat{A}$ can be expressed in terms of operators $\hat{A}$ and $\hat{\rho}$ on the smaller Hilbert space $\mathcal{H}$ only. We also call $\hat{\rho}$ the state of the system.

In general, we call any operator a density operator if it satisfies all of the following properties:

$$\hat{\rho} = \hat{\rho}^\dagger, \qquad \text{(Hermitian)} \tag{G.3}$$

$$\langle\psi| \hat{\rho} |\psi\rangle \geq 0 \quad \forall |\psi\rangle \in \mathcal{H}, \qquad \text{(positive-semidefinite)} \tag{G.4}$$

$$\operatorname{tr} \hat{\rho} = 1. \qquad \text{(unit trace)} \tag{G.5}$$

Exercise G.1. Prove that Eq. (G.2) is a density operator, i.e., it satisfies Eqs. (G.3)–(G.5).

G.1.1. Purification. A fundamental converse of Eq. (G.2) called the purification theorem says that, given any density operator $\hat{\rho}$, there exists a pure state $|\Psi\rangle$ in some larger Hilbert space $\mathcal{H} \otimes \mathcal{H}_B$ such that the right-hand side of Eq. (G.2) is equal to the given $\hat{\rho}$. $|\Psi\rangle$ is called a purification of $\hat{\rho}$. Beware that, given a $\hat{\rho}$, the purification may not be unique; there may be many purifications that give the same $\hat{\rho}$.

Remark G.1. *The term purification here does not mean any physical act of purifying something, like purifying water or turning a mixed state to a pure state. It merely means the mathematical task of finding a pure state $|\Psi\rangle$ that results in the given density operator $\hat{\rho}$ upon the partial trace.*

Exercise G.2. Given a purification $|\Psi\rangle$ of $\hat{\rho}$, prove that

$$\hat{I} \otimes \hat{U} |\Psi\rangle \tag{G.6}$$

is also a purification, where $\hat{U}$ is any unitary operator on $\mathcal{H}_B$.

G.2. Generalized Born's rule

G.2.1. Projection-valued measure (PVM). For any Hilbert space, including infinite-dimensional ones, we can use one concept called the projection-valued measure (PVM) to model all the measurement types discussed in Sec. D.2. Let Ω be the sample space for the measurement outcome and E an associated event space (see Appendix C); we often write them together as (Ω, E). A projection-valued measure $\hat{\Pi}$ takes any event $S \in E$ as an argument and produces an operator $\hat{\Pi}(S)$, such that the probability $P[S]$ of the event S is given by the formula

$$P[S] = \mathrm{tr}\left[\hat{\Pi}(S)\hat{\rho}\right], \tag{G.7}$$

where $\hat{\rho}$ is the density operator in the Schródinger picture. A measurement that can be modeled by a PVM is called a projective measurement.

$\hat{\Pi}$ is called projection-valued because $\hat{\Pi}(S)$ for any S is a projection operator, namely, it satisfies

$$\forall S \in E: \quad \hat{\Pi}(S)^\dagger = \hat{\Pi}(S), \qquad\qquad \hat{\Pi}(S)^2 = \hat{\Pi}(S). \tag{G.8}$$

Further properties of $\hat{\Pi}$ ensure that P is a probability measure satisfying the Kolmogorov axioms in Sec. C.1, such as

$$\hat{\Pi}(\Omega) = \hat{I}, \qquad\qquad \hat{\Pi}(S_1 \cup S_2) = \hat{\Pi}(S_1) + \hat{\Pi}(S_2) \quad \text{if } S_1 \cap S_2 = \varnothing. \tag{G.9}$$

An additional property is

$$\hat{\Pi}(S_1)\hat{\Pi}(S_2) = \hat{\Pi}(S_2)\hat{\Pi}(S_1) = \hat{\Pi}(S_1 \cap S_2). \tag{G.10}$$

Examples:

(1) Simple measurement with respect to orthonormal basis $\{|e_n\rangle\}$. Then $\Omega = \{1, \ldots, N\}$,

$$\hat{\Pi}(n) = |e_n\rangle \langle e_n|, \qquad\qquad \hat{\Pi}(S) = \sum_{n \in S} |e_n\rangle \langle e_n|. \tag{G.11}$$

(2) von Neumann measurement of $\hat{A} = \sum_n \lambda_n |e_n\rangle \langle e_n|$. Then $\Omega = \{\lambda_n\}$ is the set of eigenvalues,

$$\hat{\Pi}(\lambda) = \sum_{n:\lambda_n = \lambda} |e_n\rangle \langle e_n|, \qquad\qquad \hat{\Pi}(S) = \sum_{n:\lambda_n \in S} |e_n\rangle \langle e_n|. \tag{G.12}$$

(3) von Neumann measurement of continuous variable $\hat{A} = \int \lambda |A = \lambda\rangle \langle A = \lambda| \, d\lambda$. Then $\Omega = \mathbb{R}$,

$$\hat{\Pi}(S) = \int_{\lambda \in S} |A = \lambda\rangle \langle A = \lambda| \, d\lambda. \tag{G.13}$$

Exercise G.3. Show that, if $\hat{\Pi}$ is a PVM, then its Heisenberg picture defined by

$$\hat{\Pi}(S, t) \equiv \hat{U}^\dagger(t)\hat{\Pi}(S)\hat{U}(t), \quad S \in E \tag{G.14}$$

where $\hat{U}$ is a unitary operator, is also a PVM, i.e., it satisfies Eqs. (G.8)–(G.10).

For a finite-dimensional Hilbert space, the PVM concept is an overkill compared with the simple measurement in terms of an orthonormal basis, but it becomes the preferred choice of mathematicians when dealing with a continuous observable on an infinite-dimensional space, to avoid the heuristic Dirac trick.

G.2.2. Positive operator-valued measure (POVM). As discussed in Chap. 8, the most general type of measurement may enlist an ancilla for help. To model any kind of measurement, including ancilla-assisted measurements as well as projective measurements, We can use an elegant concept called the positive operator-valued measure (POVM).

Let the Schrödinger-picture density operator of a system in state $\hat{\rho}$ augmented by an ancilla in state $\hat{\rho}_B$ be $\hat{\rho} \otimes \hat{\rho}_B$ on the joint Hilbert space $\mathcal{H} \otimes \mathcal{H}_B$. The probability measure for the outcome from a projective measurement of the augmented system is

$$P[S] = \mathrm{tr}\left[\hat{\Pi}(S)(\hat{\rho} \otimes \hat{\rho}_B)\right], \tag{G.15}$$

where $\hat{\Pi}$ is the PVM on $\mathcal{H} \otimes \mathcal{H}_B$ that models the measurement. The formula can be rewritten as

$$P[S] = \mathrm{tr}\left[\hat{\Pi}(S)(\hat{\rho} \otimes \hat{\rho}_B)\right] = \mathrm{tr}\left[\hat{\Pi}(S)\Big(\hat{I} \otimes \hat{\rho}_B\Big)\Big(\hat{\rho} \otimes \hat{I}_B\Big)\right] = \boxed{\mathrm{tr}\left[\hat{M}(S)\hat{\rho}\right],} \tag{G.16}$$

where $\hat{I}$ is the identity operator on $\mathcal{H}$ and

$$\boxed{\hat{M}(S) = \mathrm{tr}_B\left[\hat{\Pi}(S)\Big(\hat{I} \otimes \hat{\rho}_B\Big)\right]} \tag{G.17}$$

is an operator on the smaller Hilbert space $\mathcal{H}$. $\hat{M}$ is called a POVM. Like a PVM, it takes any event $S \in E$ as an argument, although $\hat{M}(S)$ may not be a projection operator anymore.

In quantum information theory, it is common to draw the so-called quantum circuits, such as Fig. G.1, to represent the concepts. In the figure,

(1) each line represents a Hilbert space,
(2) each line is labeled by the initial state on the left,
(3) multiple lines represent the tensor product of the Hilbert spaces,
(4) time flows from left to right,
(5) and the cartoon on the right represents a measurement.

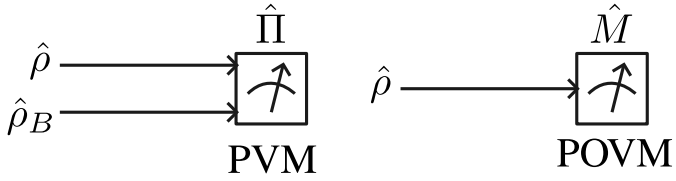

FIGURE G.1. Quantum circuits representing a measurement. Left (ancilla-assisted form): a projective measurement modeled by a PVM $\hat{\Pi}$ on a system in state $\hat{\rho}$ together with an ancilla in state $\hat{\rho}_B$. The probability distribution of the outcome is given by Eq. (G.15). Right: the same measurement can also be modeled by a POVM given by Eq. (G.17).

In general, we call any $\hat{M}$ a POVM if it satisfies the following properties:

$$\hat{M}(S) \geq 0, \qquad \hat{M}(\Omega) = \hat{I}, \qquad \hat{M}(S_1 \cup S_2) = \hat{M}(S_1) + \hat{M}(S_2) \text{ if } S_1 \cap S_2 = \varnothing. \tag{G.18}$$

G.2.3. Naimark dilation. A fundamental converse of Eq. (G.17) called the Naimark dilation theorem says that, given any POVM that satisfies Eqs. (G.18), there exist an ancilla density operator $\hat{\rho}_B$ on some Hilbert space $\mathcal{H}_B$ and a PVM $\hat{\Pi}$ on $\mathcal{H} \otimes \mathcal{H}_B$ that satisfy Eq. (G.17) [43]. Eq. (G.17) and the converse Naimark theorem imply that any measurement, simple or generalized, can be modeled by a POVM, and conversely, any POVM has a physical implementation using an ancilla, at least in principle.

While it is nice to know that any POVM is physically realizable, finding a physical setup to do it in practice is a much harder problem.

Exercise G.4. Show that a PVM is a special case of a POVM. Find an example of a POVM that is not a PVM.

Exercise G.5. Show that the Heisenberg picture of a POVM is still a POVM.

Exercise G.6. Show that homodyne detection, introduced in Chap. 8, can be modeled by a PVM, while dual-homodyne detection and heterodyne detection are examples of ancilla-assisted measurements. Find $\hat{\Pi}$, $\hat{\rho}_B$, and $\hat{M}$ for the three measurements.

G.3. Decoherence

G.3.1. Trace-preserving completely positive (TPCP) map. In Chap. 7, we considered optical loss in terms of a two-input-two-output beam-splitter model. This model turns out to be a representative example of **decoherence**, which can be defined as an interaction of a system with an inaccessible environment.

To construct a general model of decoherence, consider again a system augmented by an ancilla with a joint state $\hat{\rho} \otimes \hat{\rho}_B$ on the joint Hilbert space $\mathcal{H} \otimes \mathcal{H}_B$. (In the context of decoherence, the ancilla is not really helping us with anything, so it is more commonly called an environment, a bath, or a reservoir, although we mostly stick with the term ancilla from now on for consistency.) Suppose that the augmented system evolves in time according to a unitary operator $\hat{U}$ on $\mathcal{H} \otimes \mathcal{H}_B$, so that the final-time Schrödinger-picture state is

$$\hat{U}(\hat{\rho} \otimes \hat{\rho}_B)\hat{U}^\dagger. \tag{G.19}$$

Now we make a new decomposition of the joint Hilbert space as

$$\mathcal{H} \otimes \mathcal{H}_B \sim \mathcal{H}_C \otimes \mathcal{H}_D, \tag{G.20}$$

where $\sim$ denotes an isomorphic relation (see Sec. B.9), and assume that $\mathcal{H}_C$ is accessible while $\mathcal{H}_D$ is inaccessible at the final time. We make this new decomposition for generality—we see in Chap. 7 that, for optical loss, the accessible Hilbert space at the final time is the output mode, which lives in a different Hilbert space than that of the accessible input mode. Of course, depending on the problem, we can also take $\mathcal{H}_C = \mathcal{H}$ and $\mathcal{H}_D = \mathcal{H}_B$.

We call the state on $\mathcal{H}_C$ at the final time the final system state. It is given by the partial trace

$$\boxed{\mathrm{tr}_D\left[\hat{U}(\hat{\rho} \otimes \hat{\rho}_B)\hat{U}^\dagger\right] \equiv \mathcal{F}\hat{\rho}.} \tag{G.21}$$

This relation defines a map $\mathcal{F}$ from the initial system state $\hat{\rho}$ on $\mathcal{H}$ to the final system state on $\mathcal{H}_C$. $\mathcal{F}$ is called a trace-preserving completely positive (TPCP) map. Some quantum circuits representing Eq. (G.21) are shown in Fig. G.2.

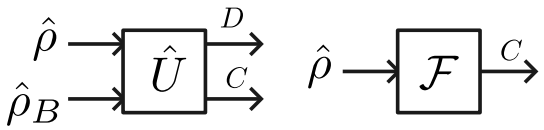

FIGURE G.2. Quantum circuits representing a trace-perserving completely positive (TPCP) map given by Eq. (G.21). The label x on top of each line indicates that the Hilbert space represented by the line is $\mathcal{H}_x$. The left figure is the ancilla-assisted form and the right figure is the simplified form.

Let $\mathcal{O}(\mathcal{H})$ be the space of operators on a Hilbert space $\mathcal{H}$. Then the domain of $\mathcal{F}$ is $\mathcal{O}(\mathcal{H})$, the codomain is $\mathcal{O}(\mathcal{H}_C)$, and we write $\mathcal{F} : \mathcal{O}(\mathcal{H}) \to \mathcal{O}(\mathcal{H}_C)$. Such a map is sometimes called a superoperator, as it is an operator on operators.

$\mathcal{F}$ in Eq. (G.21) is trace preserving because

$$\mathrm{tr}\,(\mathcal{F}\hat{\rho}) = \mathrm{tr}_C\,\mathrm{tr}_D\left[\hat{U}(\hat{\rho} \otimes \hat{\rho}_B)\hat{U}^\dagger\right] = \mathrm{tr}\left[\hat{U}(\hat{\rho} \otimes \hat{\rho}_B)\hat{U}^\dagger\right] = (\mathrm{tr}\,\hat{\rho})(\mathrm{tr}\,\hat{\rho}_B) = \mathrm{tr}\,\hat{\rho}, \tag{G.22}$$

where we have assumed $\mathrm{tr}\,\hat{\rho}_B = 1$. In other words, the trace of the final system state is equal to the trace of the initial system state $\hat{\rho}$. We demand $\mathrm{tr}\,\hat{\rho} = 1$ for a density operator, so $\mathrm{tr}(\mathcal{F}\hat{\rho}) = 1$ is satisfied if $\mathcal{F}$ is trace preserving.

Side note. *The "completely positive" (CP) part of the name refers to a certain mathematical property of the map* https://en.wikipedia.org/wiki/Completely_positive_map. *To describe this property, let $\mathcal{H}_n$ be yet another Hilbert space with dimension $n < \infty$ and $\mathcal{O}(\mathcal{H} \otimes \mathcal{H}_n)$ be the space of operators on $\mathcal{H} \otimes \mathcal{H}_n$. We define a new map $\mathcal{F} \otimes \mathcal{I}_n : \mathcal{O}(\mathcal{H} \otimes \mathcal{H}_n) \to \mathcal{O}(\mathcal{H}_C \otimes \mathcal{H}_n)$ by*

$$(\mathcal{F} \otimes \mathcal{I}_n)(\hat{A} \otimes \hat{B}) \equiv \left(\mathcal{F}\hat{A}\right) \otimes \hat{B} \in \mathcal{O}(\mathcal{H}_C \otimes \mathcal{H}_n). \tag{G.23}$$

This relation for any $\hat{A} \otimes \hat{B}$ is enough to define $\mathcal{F} \otimes \mathcal{I}_n : \mathcal{O}(\mathcal{H} \otimes \mathcal{H}_n) \to \mathcal{O}(\mathcal{H}_C \otimes \mathcal{H}_n)$ in general. Now a CP map is defined as a map $\mathcal{F}$ such that, for any $n < \infty$, $\mathcal{F} \otimes \mathcal{I}_n$ maps positive-semidefinite operators in $\mathcal{O}(\mathcal{H} \otimes \mathcal{H}_n)$ to positive-semidefinite operators in $\mathcal{O}(\mathcal{H}_C \otimes \mathcal{H}_n)$.

Physically, this CP property together with the trace-preserving property imply that the application of the map $\mathcal{F} \otimes \mathcal{I}_n$ on a density operator on any larger Hilbert space should give another density operator.

If the definition of the CP property sounds too complicated for your taste, I don't blame you—we don't actually use the definition much in physics. Instead, we usually think of a CP map as a shorthand for the left-hand side of Eq. (G.21).

G.3.2. Kraus form. There's a more succinct way of writing a TPCP map called a Kraus form or a Kraus representation. First write the ancilla state $\hat{\rho}_B$ in the diagonal form

$$\hat{\rho}_B = \sum_n p_n |e_n\rangle \langle e_n| , \tag{G.24}$$

where $\{p_n\}$ are some positive numbers and $\{|e_n\rangle\}$ are a set of vectors in $\mathcal{H}_B$. Write also the identity operator $\hat{I}_D$ on $\mathcal{H}_D$ as a completeness relation

$$\hat{I}_D = \sum_m |f_m\rangle \langle f_m| \tag{G.25}$$

in terms of a set of vectors $\{|f_m\rangle\}$ in $\mathcal{H}_D$. Then we can write the TPCP map as

$$\boxed{\mathcal{F}\hat{\rho} = \sum_{m,n} \hat{K}_{mn} \hat{\rho} \hat{K}_{mn}^\dagger,} \tag{G.26}$$

where

$$\boxed{\hat{K}_{mn} \equiv \sqrt{p_n} \langle f_m| \hat{U} |e_n\rangle} \tag{G.27}$$

is an operator $\hat{K}_{nm} : \mathcal{H} \to \mathcal{H}_C$ called a **Kraus operator**. $\langle f_m|$ and $|e_n\rangle$ in Eq. (G.27) should be interpreted as a partial bra and a partial ket, respectively (see Sec. B.10). The expression of a map in the form of Eq. (G.26), where we sandwich the initial system state $\hat{\rho}$ between two operators $\hat{K}_{mn}$ and $\hat{K}_{mn}^\dagger$ and then take the sum, is called a Kraus form or an operator-sum form.

Beware that the Kraus form of a TPCP map may not be unique, i.e., there may be many sets of operators that give the same CP map $\mathcal{F}$. For example, the diagonal form of $\hat{\rho}_B$ given by Eq. (G.24) and the completeness relation given by Eq. (G.25) may not be unique, so the Kraus operators $\{\hat{K}_{mn}\}$ are different depending on the forms we choose. By virtue of the purification theorem, we can also assume a pure ancilla state $\hat{\rho}_B = |\psi\rangle \langle\psi|$ on a large enough Hilbert space, so that a Kraus operator becomes

$$\hat{K}_m = \langle f_m| \hat{U} |\psi\rangle \tag{G.28}$$

with only one index.

G.3.3. Stinespring dilation. In general, any map $\mathcal{F}$ in the Kraus form

$$\mathcal{F}\hat{\rho} \equiv \sum_m \hat{K}_m \hat{\rho} \hat{K}_m^\dagger \tag{G.29}$$

for some Kraus operators $\{\hat{K}_m\}$ can be shown to be CP. A fundamental converse of Eq. (G.29) called the Stinespring dilation theorem says that, if a map $\mathcal{F}$ is CP, then it can always be expressed in a Kraus form for some Kraus operators $\{\hat{K}_m\}$. If the map is also trace preserving, then the Kraus operators must also satisfy

$$\sum_m \hat{K}_m^\dagger \hat{K}_m = \hat{I}. \tag{G.30}$$

It turns out that, given a set of Kraus operators that satisfy Eq. (G.30), one can always cook up an ancilla state $\hat{\rho}_B = |\psi\rangle \langle\psi|$ and some unitary operator $\hat{U}$ so that Eq. (G.28) holds and the map can be written in an ancilla-assisted

form on the left-hand side of Eq. (G.21) [46, Theorem 5.1]. In other words, any TPCP map is physically realizable, at least in principle.

G.4. Time evolution

G.4.1. Quantum Markov chain. For a system that interacts with n ancillas sequentially, the final system state in the Schrödinger picture can be expressed as sequential applications of TPCP maps $\mathcal{F}_1, \mathcal{F}_2 \ldots, \mathcal{F}_n$:

$$\boxed{\hat{\rho}_n = \mathcal{F}_n \ldots \mathcal{F}_2 \mathcal{F}_1 \hat{\rho}_0,} \tag{G.31}$$

where $\hat{\rho}_0$ is the initial state on a Hilbert space $\mathcal{H}_0$ and $\mathcal{F}_j : \mathcal{O}(\mathcal{H}_{j-1}) \to \mathcal{O}(\mathcal{H}_j)$. Each TPCP map can be expressed as

$$\mathcal{F}_j \hat{\rho}_{j-1} = \mathrm{tr}_{D_j} \left[\hat{U}_j (\hat{\rho}_{j-1} \otimes \hat{\sigma}_j) \hat{U}_j^\dagger \right], \tag{G.32}$$

where $\hat{\sigma}_j$ is an ancilla state on $\mathcal{H}_{B_j}$, $\hat{U}_j$ is a unitary operator on $\mathcal{H}_{j-1} \otimes \mathcal{H}_{B_j}$, we assume

$$\mathcal{H}_{j-1} \otimes \mathcal{H}_{B_j} \sim \mathcal{H}_j \otimes \mathcal{H}_{D_j}, \tag{G.33}$$

and tr_{D_j} is the partial trace with respect to $\mathcal{H}_{D_j}$. Some quantum circuits representing Eqs. (G.31) and (G.32) are shown in Fig. G.3.

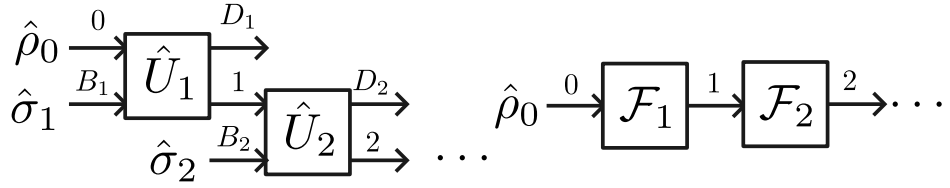

FIGURE G.3. Quantum circuits representing the quantum Markov chain modeled by Eqs. (G.31) and (G.32). The left figure is the ancilla-assisted form and the right figure is the simplified form.

Physically, Eqs. (G.31) and (G.32) imply that, at each time step, the ancilla is always in a fresh state $\hat{\sigma}_j$ independent of the system and the other ancillas for the other time steps.

Another perspective is to think of the n ancillas as one big bath. Then Eqs. (G.31) and (G.32) imply that the bath "forgets" any previous interaction with the system and becomes independent of the system at the beginning of each time step.

We call Eq. (G.31) a Markov chain because it is a generalization of the classical Markov chain. Let $(X_0, X_1, \ldots, X_n)$ be a classical random process with discrete time $j = 0, 1, \ldots, n$. Assume also countable sample spaces for simplicity. The probability distribution of X_n can be expressed as

$$\begin{aligned} P_{X_n}(x_n) = \sum_{x_{n-1},\ldots,x_0} & P_{X_n|X_{n-1},\ldots,X_0}(x_n|x_{n-1},\ldots,x_0) P_{X_{n-1}|X_{n-2},\ldots,X_0}(x_{n-1}|x_{n-2},\ldots,x_0) \ldots \\ & P_{X_1|X_0}(x_1|x_0) P_{X_0}(x_0). \end{aligned} \tag{G.34}$$

Make the Markov approximation

$$P_{X_j|X_{j-1},\ldots,X_0}(x_j|x_{j-1},\ldots,x_0) = P_{X_j|X_{j-1}}(x_j|x_{j-1}), \tag{G.35}$$

which means that each $P_{X_j|X_{j-1},\ldots,X_0}$ depends only on the immediate previous value X_{j-1} and "forgets" the earlier values. Then we can write

$$P_{X_n} = \sum_{x_{n-1}} P_{X_n|X_{n-1}}(x_n|x_{n-1}) \cdots \sum_{x_1} P_{X_2|X_1}(x_2|x_1) \sum_{x_0} P_{X_1|X_0}(x_1|x_0) P_{X_0}(x_0). \tag{G.36}$$

We can now think of each operation

$$P_{X_j}(x_j) = \sum_{x_{j-1}} P_{X_j|X_{j-1}}(x_j|x_{j-1}) P_{X_{j-1}}(x_{j-1}) \tag{G.37}$$

as a map from a distribution $P_{X_{j-1}}$ to another distribution P_{X_j}; each $\mathcal{F}_j$ in Eq. (G.31) is a generalization of such a map. The "Markovianity" in the quantum case comes from the independent ancilla assumed in each time step.

G.4.2. Master equation. Let

$$t_j = t_0 + j\Delta t, \quad j = 0, 1, 2, \ldots, \tag{G.38}$$

be the discrete time with step size Δt,

$$\hat{\rho}(t_j) = \hat{\rho}_j \tag{G.39}$$

be the Schrödinger-picture density operator of the system at time t_j, and assume that the system at each time always lives on the same Hilbert space $\mathcal{H}$, so that $\mathcal{F}_j : \mathcal{O}(\mathcal{H}) \to \mathcal{O}(\mathcal{H})$. Write the map as

$$\mathcal{F}_j = \exp[\mathcal{L}(t_j)\Delta t], \tag{G.40}$$

where $\mathcal{L}(t_j) : \mathcal{O}(\mathcal{H}) \to \mathcal{O}(\mathcal{H})$ is another map and Δt is the duration of the time step. In the limit $\Delta t \to 0$, we can model the time evolution in Eq. (G.31) in the form of a differential equation

$$\boxed{\frac{d\hat{\rho}(t)}{dt} = \lim_{\Delta t \to 0} \frac{\hat{\rho}(t_j) - \hat{\rho}(t_{j-1})}{\Delta t} = \mathcal{L}(t)\hat{\rho}(t).} \tag{G.41}$$

This equation is called a (Markovian) master equation. In the continuous-time limit, we can write $\mathcal{F}_n \ldots \mathcal{F}_1$ formally as

$$\mathcal{F}_n \ldots \mathcal{F}_1 \to \mathcal{T} \exp\left[\int_0^{t_n} \mathcal{L}(t)dt\right] \equiv \mathcal{G}(t_n), \tag{G.42}$$

where $\mathcal{T}$ denotes time ordering (https://en.wikipedia.org/wiki/Path-ordering#Time_ordering). If $\mathcal{L}(t)$ does not depend on time, the set $\mathcal{G} \equiv \{\mathcal{G}(t) : t \geq 0\}$ is called a quantum Markov semigroup, and we can write each element of the semigroup as

$$\mathcal{G}(t) = \exp(\mathcal{L}t), \tag{G.43}$$

where $\mathcal{L}$ is called the generator of the semigroup. $\mathcal{G}(t)$ for each t is a TPCP map, and $\mathcal{G}$ is called a semigroup because of the property $\mathcal{G}(t)\mathcal{G}(t') = \mathcal{G}(t + t')$. $\mathcal{G}$ is only a semigroup, not a group, because the set $\mathcal{G}$ may not contain the inverse of each $\mathcal{G}(t)$.

Gorini, Kossakowski, Sudarshan [49], and Lindblad [50] (GKSL) found that the generator of any quantum Markov semigroup can be expressed as

$$\boxed{\mathcal{L}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_j \gamma_j \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2}\hat{L}_j^\dagger \hat{L}_j \hat{\rho} - \frac{1}{2}\hat{\rho}\hat{L}_j^\dagger \hat{L}_j\right),} \tag{G.44}$$

where $\hat{H}$ is a Hamiltonian, each γ_j is a positive real constant, and each $\hat{L}_j$ is called a jump operator. Conversely, as long as $\hat{H}$ is Hermitian and each γ_j is positive, the right-hand side is the generator of some quantum Markov semigroup.

Beware that the GKSL form is not unique, i.e., there exist many different Hamiltonians and jump operators that give the same generator $\mathcal{L}$.

The quantum Markovian master equation generalizes the Fokker-Planck equation and the Chapman-Kolmogorov equation in the classical case [51].

Remark G.2. *To model time evolution using multiple TPCP maps $\mathcal{F}_n \ldots \mathcal{F}_1$, Δt for each $\mathcal{F}_j$ needs to be long enough for the bath to forget the interaction and begin in a fresh ancilla state for the next map. Yet, here we have taken the limit of $\Delta t \to 0$ to derive the master equation. It is therefore important to keep in mind that the master equation, while mathematically well defined, is an approximation of the fundamental physics. It does model many phenomena quite well, such as the Brownian motion, but may cease to be accurate when the physics becomes "non-Markovian."*

The fundamental dynamics of a closed system (i.e., no ancilla) is described by the Liouville equation in the classical case or the Schrödinger equation in the quantum case, and we do get precise Markovianity. For any other

open system, however, Markovianity is an approximation, not a clear-cut property. It can get more or less accurate depending on how we make the system-ancilla partition.

Side note. *The right-hand side of Eq. (G.44) is often called the Lindblad generator or Lindbladian, while the master equation in terms of the right-hand side of Eq. (G.44) is often called the Lindblad master equation, but that would not be fair to GKS, who discovered the form independently at around the same time.*

G.5. Indirect measurement

Suppose that a system with initial state $\hat{\rho}$ interacts with an ancilla with initial state $\hat{\rho}_B$ through a unitary operator $\hat{U}$. Then we perform a partial measurement in terms of a POVM $\hat{M}_D$ on $\mathcal{H}_D$ only, with sample and event spaces (Ω, E). This measurement scheme is called an indirect measurement. For example, we often measure an atomic or solid-state system by sending an optical probe beam with multiple modes to interact with the system, before measurements of the output optical modes.

With an indirect measurement, the measurement on the ancilla can be destructive while the system remains intact, so we can study what happens to the system after the measurement. The central concept for this problem is the **hybrid state**, defined as

$$\boxed{\mathrm{tr}_D\left\{\left[\hat{I}_C \otimes \hat{M}_D(S)\right]\hat{U}(\hat{\rho}\otimes\hat{\rho}_B)\hat{U}^\dagger\right\} \equiv \mathcal{F}(S)\hat{\rho},} \quad S \in E, \tag{G.45}$$

where $\hat{I}_s$ for any subscript s is the identity operator on $\mathcal{H}_s$. We call $\mathcal{F} : E \times \mathcal{O}(\mathcal{H}) \to \mathcal{O}(\mathcal{H}_C)$ a map-valued measure, since $\mathcal{F}(S) : \mathcal{O}(\mathcal{H}) \to \mathcal{O}(\mathcal{H}_C)$ for each event S is a CP map, while $\mathcal{F}(S)\hat{\rho}$ for each S is a positive-semidefinite operator on $\mathcal{H}_C$. The probability of S becomes

$$P[S] = \mathrm{tr}\left[\mathcal{F}(S)\hat{\rho}\right], \tag{G.46}$$

while the unconditional quantum state on $\mathcal{H}_C$ if we ignore the measurement outcome is $\mathcal{F}(\Omega)\hat{\rho}$, where $\mathcal{F}(\Omega)$ is a TPCP map. The normalization condition for the hybrid state is hence

$$\mathrm{tr}\left[\mathcal{F}(\Omega)\hat{\rho}\right] = \mathrm{tr}\,\hat{\rho} = 1. \tag{G.47}$$

$\mathcal{F}(S)\hat{\rho}$ behaves like a joint probability distribution, except that one part is classical and one part is quantum (hence the name hybrid state). It gives a classical probability measure if we ignore the quantum part by taking the trace and gives a quantum density operator if we ignore the classical part by plugging $S = \Omega$.

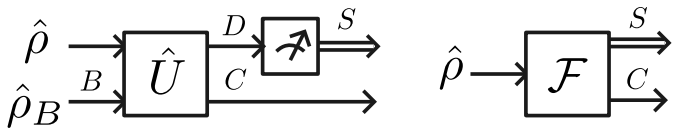

FIGURE G.4. Quantum circuits representing Eq. (G.45) for the hybrid state $\mathcal{F}(S)\hat{\rho}$ produced by an indirect measurement. A double line represents a classical variable and the symbol on top is the event S. The left figure is the ancilla-assisted form and the right figure is the simplified form.

We can write Eq. (G.45) in the Kraus form as well. First rewrite $\hat{M}_D(S)$ in terms of its square root (see Sec. B.6) as

$$\hat{M}_D(S) = \sqrt{\hat{M}_D(S)}\sqrt{\hat{M}_D(S)}, \qquad \hat{I}_C \otimes \hat{M}_D(S) = \left[\hat{I}_C \otimes \sqrt{\hat{M}_D(S)}\right]\left[\hat{I}_C \otimes \sqrt{\hat{M}_D(S)}\right]. \tag{G.48}$$

Then we can use the cyclic property of the partial trace given by Eq. (B.122) to write

$$\mathcal{F}(S)\hat{\rho} = \mathrm{tr}_D\left\{\left[\hat{I}_C \otimes \sqrt{\hat{M}_D(S)}\right]\hat{U}(\hat{\rho}\otimes\hat{\rho}_B)\hat{U}^\dagger\left[\hat{I}_C \otimes \sqrt{\hat{M}_D(S)}\right]\right\} = \sum_{m,n}\hat{K}_{mn}(S)\hat{\rho}\hat{K}_{mn}(S)^\dagger, \tag{G.49}$$

where the Kraus operator

$$\hat{K}_{mn}(S) \equiv \sqrt{p_n} \langle f_m | \left[\hat{I}_C \otimes \sqrt{\hat{M}_D(S)} \right] \hat{U} | e_n \rangle \tag{G.50}$$

generalizes Eq. (G.27).

G.6. Posterior state

Let the first measurement outcome be X. If we make another measurement on the system with POVM $\hat{M}_C$ on $\mathcal{H}_C$ and the outcome is Y, the joint probability of $Y \in R$ and $X \in S$ becomes

$$\boxed{P[(Y \in R) \text{ and } (X \in S)] = \operatorname{tr}\left[\hat{M}_C(R) \mathcal{F}(S) \hat{\rho} \right].} \tag{G.51}$$

The probability of $Y \in R$ conditioned on $X \in S$ is then

$$P[Y \in R | X \in S] \equiv \frac{P[(Y \in R) \text{ and } (X \in S)]}{P[X \in S]} = \frac{\operatorname{tr}\left[\hat{M}_C(R) \mathcal{F}(S) \hat{\rho} \right]}{\operatorname{tr}\left[\mathcal{F}(S) \hat{\rho} \right]}. \tag{G.52}$$

Hence, we can regard

$$\boxed{\hat{\rho}_S \equiv \frac{\mathcal{F}(S) \hat{\rho}}{\operatorname{tr}\left(\text{numerator} \right)}} \tag{G.53}$$

as the posterior system state conditioned on the event $X \in S$, so that any subsequent measurement can be modeled as

$$P[Y \in R | X \in S] = \operatorname{tr}\left[\hat{M}_C(R) \hat{\rho}_S \right]. \tag{G.54}$$

Eq. (G.53) is sometimes called a quantum Bayes theorem. It generalizes the phenomenon of measurement-induced collapse in ordinary quantum mechanics.

Side note. *There are many proposals to generalize Bayes theorem in quantum mechanics; Eq. (G.53) is only one special case.*

We can also condition on a measurement outcome $X = x$. This is most easily done if X is discrete: just take $S = x$, so that the posterior state becomes

$$\hat{\rho}_x = \frac{\mathcal{F}(x) \hat{\rho}}{\operatorname{tr}\left(\text{numerator} \right)}, \quad x \in \Omega. \tag{G.55}$$

If X is continuous, however, the definition of a posterior state is a bit trickier, similar to the classical problem in Sec. C.4. To proceed, we assume that the POVM in Eq. (G.45) can be expressed as

$$\hat{M}_D(S) = \int_{x \in S} \hat{f}_D(x) d\mu(x) \tag{G.56}$$

for a classical reference measure μ and an operator-valued density $\hat{f}_D : \Omega \to \mathcal{O}(\mathcal{H}_D)$. Then we can think of the POVM as a function of the outcome x as

$$\hat{M}_D(x) = \hat{f}_D(x) d\mu(x). \tag{G.57}$$

For example, for a von Neumann measurement of $\hat{A} = \int x \, |A = x\rangle \langle A = x| \, dx$, we can use the Dirac trick to write

$$\hat{M}_D(S) = \int_{x \in S} |A = x\rangle \langle A = x| \, dx, \qquad \hat{M}_D(x) = |A = x\rangle \langle A = x| \, dx. \tag{G.58}$$

Given $\hat{f}_D(x)$, we write $\mathcal{F}(x)$ for an outcome x as

$$\mathcal{F}(x) = d\mu(x) \underbrace{\operatorname{tr}_D \left\{ \left[\hat{I}_C \otimes \hat{f}_D(x) \right] \hat{U} (\hat{\rho} \otimes \hat{\rho}_B) \hat{U}^\dagger \right\}}_{\equiv \mathsf{f}(x) \hat{\rho}}, \tag{G.59}$$

so that

$$\mathrm{tr}\left[\mathcal{F}(x)\hat{\rho}\right] = d\mu(x)\,\mathrm{tr}\left[\mathsf{f}(x)\hat{\rho}\right] \tag{G.60}$$

and $\mathrm{tr}[\mathsf{f}(x)\hat{\rho}]$ gives the probability density. The posterior state becomes

$$\hat{\rho}_x = \frac{\mathcal{F}(x)\hat{\rho}}{\mathrm{tr}[\mathcal{F}(x)\hat{\rho}]} = \frac{\mathsf{f}(x)\hat{\rho}}{\mathrm{tr}[\mathsf{f}(x)\hat{\rho}]}, \tag{G.61}$$

where $d\mu(x)$ drops out of the final expression.

G.7. Sequential measurements

We can model sequential measurements with outcomes $(X_1, \ldots, X_n) \in \Omega_1 \times \cdots \times \Omega_n$ by assuming the hybrid state

$$\boxed{\mathcal{F}(S_n, \ldots, S_1)\hat{\rho} = \mathcal{F}_n(S_n)\ldots\mathcal{F}_1(S_1)\hat{\rho},} \tag{G.62}$$

where $\hat{\rho}$ is the initial system state, each $\mathcal{F}_j$ is a map-valued measure in the form of Eq. (G.45), and each S_j is an event for the jth measurement outcome X_j. Each $\mathcal{F}_j$ can also model any time evolution and decoherence besides the measurement by including additional degrees of freedom in the ancilla and modifying the ancilla state and the unitary in Eq. (G.45) accordingly. The joint probability of all the events becomes

$$P[(X_n \in S_n) \text{ and } \ldots \text{ and } (X_1 \in S_1)] = \mathrm{tr}\left[\mathcal{F}_n(S_n)\ldots\mathcal{F}_1(S_1)\hat{\rho}\right]. \tag{G.63}$$

If we ignore all the outcomes and plug the sample space Ω_j for each outcome into S_j, we get back the Markov chain in Sec. G.4.1:

$$\hat{\rho}_n = \mathcal{F}_n(\Omega_n)\ldots\mathcal{F}_1(\Omega_1)\hat{\rho}. \tag{G.64}$$

We can also compute the posterior state by

$$\hat{\rho}_{S_n,\ldots,S_1} \equiv \frac{\mathcal{F}_n(S_n)\ldots\mathcal{F}_1(S_1)\hat{\rho}}{\mathrm{tr}\,(\text{numerator})}, \tag{G.65}$$

or by the iterative relation

$$\hat{\rho}_{S_j,\ldots,S_1} = \frac{\mathcal{F}_j(S_j)\hat{\rho}_{S_{j-1},\ldots,S_1}}{\mathrm{tr}(\text{numerator})} \tag{G.66}$$

for the posterior state $\hat{\rho}_{S_j,\ldots,S_1}$ at each time. Fig. G.5 shows some quantum circuits representing Eq. (G.63).

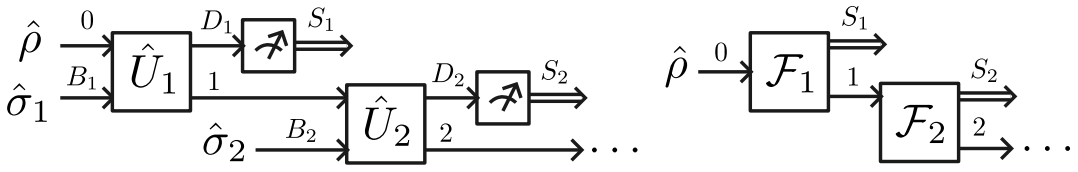

FIGURE G.5. Quantum circuits representing sequential measurements modeled by Eq. (G.63). The left figure is the ancilla-assisted form and the right figure is the simplified form.

G.8. Continuous measurement

The outcomes of sequential measurements form a discrete-time random process $(X_1, \ldots, X_n)$. There is a beautiful theory of continuous measurement, pioneered by Belavkin, that takes the continuous-time limit of the sequential-measurement model, so that the outcomes become a continuous-time random process [45]. The resulting equation for the posterior state is called a stochastic master equation, a generalization of the master equation we introduced in Sec. G.4.2.

The stochastic master equation is less popular and arguably less useful, however, because

(1) It requires stochastic calculus, a hairy subject.

(2) It isn't any easier to solve than the discrete-time Eqs. (G.65) or (G.66) in most cases. One often needs to solve the stochastic master equation numerically assuming discrete time, but then one may as well solve Eqs. (G.65) or (G.66) without ever worrying about stochastic calculus.
(3) Outcomes from real-life measurements are always recorded at discrete times and a continous-time process is only an approximation, so a stochastic master equation is an approximation in any case.

G.9. Measurement-based feedback

An experimenter can take the measurement outcomes and modify the future dynamics based on the outcomes. We can model measurement-based feedback by assuming that each $\mathcal{F}_j$ depends on the previous events $S_{j-1}, \ldots, S_1$. For example, consider two sequential measurements. Then the conditional probability is

$$P[S_2|S_1] = \mathrm{tr}\,[\mathcal{F}_2(S_2|S_1)\hat{\rho}_{S_1}], \qquad \hat{\rho}_{S_1} = \frac{\mathcal{F}_1(S_1)\hat{\rho}}{\mathrm{tr}(\text{numerator})}, \tag{G.67}$$

and the joint probability distribution becomes

$$P[S_2 \text{ and } S_1] = P[S_2|S_1]P[S_1] = \mathrm{tr}\,[\mathcal{F}_2(S_2|S_1)\mathcal{F}_1(S_1)\hat{\rho}]. \tag{G.68}$$

Fig. G.6 shows the quantum circuits that represent the feedback.

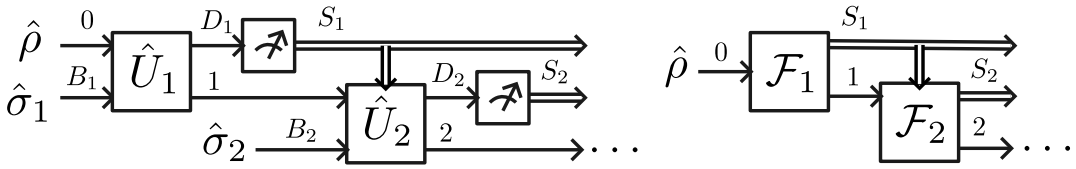

FIGURE G.6. The first event S_1 can be used to modify future dynamics by perturbing $\hat{U}_2(S_1)$ or $\mathcal{F}_2(S_2|S_1)$.

This argument can be generalized for multiple measurements, so that Eqs. (G.62)–(G.66) remain valid if each $\mathcal{F}_j(S_j)$ depends on the previous events, and we can rewrite it as $\mathcal{F}_j(S_j|S_{j-1}, \ldots, S_1)$.

G.10. Principle of deferred measurement

Similar to the theorems of purification, Naimark, and Stinespring, it turns out that, through the so-called principle of deferred measurement [47], we can also model sequential measurements and measurement-based feedback by ordinary quantum mechanics without resorting to CP maps.

To see how it works, first consider a simple example of a system on $\mathcal{H}$ and an optical mode as the ancilla on $\mathcal{H}_B$. Let the initial state of the augmented system be $\hat{\rho}$ on $\mathcal{H} \otimes \mathcal{H}_B$ and consider the following experiment:

(1) The experimenter measures the photon number $\hat{n} = \sum_n n\,|n\rangle\langle n|$ of the optical mode.
(2) The experimenter then uses the outcome n to modify the dynamics of the system, so that the unitary operator of the system after the measurement becomes a function $\hat{U}(n)$ of n.

This experiment turns out to be equivalent to the following:

(1) The system and the optical mode interact according to the so-called **controlled unitary operator**

$$\hat{V} \equiv \sum_n \hat{U}(n) \otimes |n\rangle\langle n|\,. \tag{G.69}$$

(2) Then the experimenter measures the photon number of the optical mode.

To show that the two experiments are equivalent, we observe that the hybrid state for the first experiment

$$\mathcal{F}_1(n)\hat{\rho} \equiv \hat{U}(n)\Big\{\mathrm{tr}_B\Big[\Big(\hat{I} \otimes |n\rangle\langle n|\Big)\hat{\rho}\Big]\Big\}\hat{U}(n)^\dagger \tag{G.70}$$

is equal to the hybrid state for the second experiment

$$\mathcal{F}_2(n)\hat{\rho} \equiv \mathrm{tr}_B\Big[\Big(\hat{I} \otimes |n\rangle\langle n|\Big)\hat{V}\hat{\rho}\hat{V}^\dagger\Big]. \tag{G.71}$$

With the same hybrid state $\mathcal{F}_1(n)\hat{\rho} = \mathcal{F}_2(n)\hat{\rho}$, the joint probability distribution $P(m,n) = \mathrm{tr}[\hat{M}(m)\mathcal{F}_j(n)\hat{\rho}]$ after any subsequent measurement with outcome m is the same, so the two experiments are indistinguishable. In other words, we do not have to use a CP map $\mathrm{tr}_B\left[\left(\hat{I}\otimes|n\rangle\langle n|\right)\hat{\rho}\right]$ to describe the measurement before the feedback; we can use a controlled unitary $\hat{V}$ on a larger Hilbert space to model the procedure and assume that the measurement is performed afterwards. The general idea is depicted in Fig. G.7.

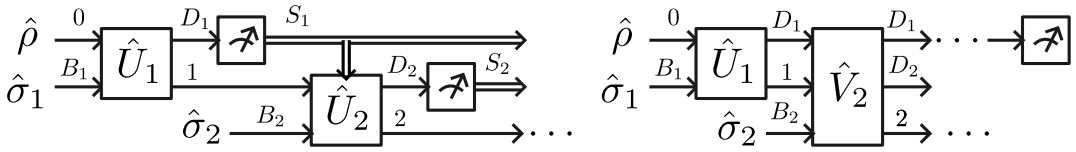

FIGURE G.7. Sequential measurements and measurement-based feedback (left) can be modeled by controlled unitaries and deferred measurements (right).

Exercise G.7. Show that $\hat{V}$ given by Eq. (G.69) is a unitary operator.

Exercise G.8. Show that Eqs. (G.70) and (G.71) are equal.

We now prove the principle for sequential measurements in general, at least for discrete outcomes and finite-dimensional Hilbert spaces.

(1) Write each map in the ancilla-assisted form as

$$\mathcal{F}_j(x_j|y_j)\hat{\rho}_{j-1} = \mathrm{tr}_{D_j}\left\{\left[\hat{I}_j\otimes\hat{\Pi}_j(x_j)\right]\hat{U}_j(y_j)(\hat{\rho}_{j-1}\otimes\hat{\sigma}_j)\hat{U}_j(y_j)^\dagger\left[\hat{I}_j\otimes\hat{\Pi}_j(x_j)\right]\right\} \tag{G.72}$$

$$= \mathrm{tr}_{D_j}\left\{\left[\hat{I}_j\otimes\hat{\Pi}_j(x_j)\right]\hat{U}_j(y_j)\,|\psi_j\rangle\,\hat{\rho}_{j-1}\,\langle\psi_j|\,\hat{U}_j(y_j)^\dagger\left[\hat{I}_j\otimes\hat{\Pi}_j(x_j)\right]\right\} \tag{G.73}$$

$$\hat{\sigma}_j = |\psi_j\rangle\langle\psi_j|, \quad y_j \equiv (x_{j-1},\ldots,x_1). \tag{G.74}$$

Note that

(a) $\hat{\rho}_j$ is on $\mathcal{H}_j$, $\hat{\sigma}_j$ is on $\mathcal{H}_{B_j}$, $\hat{U}_j$ is on

$$\mathcal{H}_{j-1}\otimes\mathcal{H}_{B_j} \sim \mathcal{H}_j\otimes\mathcal{H}_{D_j}, \tag{G.75}$$

and $\hat{\Pi}_j$ is on $\mathcal{H}_{D_j}$.

(b) In Eq. (G.73),

$$|\psi_j\rangle : \mathcal{H}_{j-1} \to \mathcal{H}_{j-1}\otimes\mathcal{H}_{B_j}, \qquad \langle\psi_j| : \mathcal{H}_{j-1}\otimes\mathcal{H}_{B_j} \to \mathcal{H}_{j-1} \tag{G.76}$$

are understood to be a partial ket and a partial bra, respectively.

(c) We have assumed a suitable ancilla so that the measurement can be modeled by a PVM $\hat{\Pi}_j$.

(d) $\hat{\sigma}_j$ can always be assumed to be pure on a large enough Hilbert space by virtue of the purification theorem.

(e) We have used $\hat{\Pi}_j(x_j) = \hat{\Pi}_j(x_j)^2$ for a PVM and the cyclic property of the partial trace given by Eq. (B.122).

(f) Without loss of generality, $|\psi_j\rangle$ can be assumed to be independent of the previous outcomes y_j. Proof: Because any two pure states can be related by a unitary operator, we can write any y_j-dependent pure state as

$$|\phi(y_j)\rangle = \hat{u}(y_j)\,|\psi_j\rangle \tag{G.77}$$

in terms of a y_j-dependent unitary $\hat{u}(y_j)$ and a fixed $|\psi_j\rangle$, and $\hat{u}(y_j)$ can be absorbed into $\hat{U}_j(y_j)$ by a redefinition of $\hat{U}_j$.

(g) With no practical loss of generality, we can also assume $\hat{\Pi}_j$ to be independent of y_j. Let's prove it for simple measurements with

$$\hat{\pi}_j(x|y_j) = |e_x(y_j)\rangle \langle e_x(y_j)|, \tag{G.78}$$

where $\{|e_x(y_j)\rangle\}$ for each y_j is an orthonormal basis of $\mathcal{H}_{D_j}$. Since two orthonormal bases of a Hilbert space can always be related by a unitary operator, we can write any PVM for a simple measurement as

$$\hat{\pi}_j(x|y_j) = |e_x(y_j)\rangle \langle e_x(y_j)| = \hat{u}(y_j) \left|e'_x\right\rangle \left\langle e'_x\right| \hat{u}(y_j)^\dagger = \hat{u}(y_j)\hat{\Pi}_j(x)\hat{u}(y_j)^\dagger \tag{G.79}$$

in terms of a y_j-dependent unitary $\hat{u}(y_j)$ and a fixed PVM $\hat{\Pi}_j(x) = |e'_x\rangle \langle e'_x|$. Then

$$\left[\hat{I}_j \otimes \hat{\pi}_j(x|y_j)\right]\hat{U}_j(y_j) = \left[\hat{I}_j \otimes \hat{u}(y_j)\hat{\Pi}_j(x)\hat{u}(y_j)^\dagger\right]\hat{U}_j(y_j), \tag{G.80}$$

the $\hat{u}(y_j)^\dagger$ on the right can be absorbed into $\hat{U}_j(y_j)$ while the $\hat{u}(y_j)$ on the left goes away after the partial trace tr_{D_j}.

Side note. *As long as we stick to a finite-dimensional Hilbert space, the proof for projective measurements is pretty much the same. For an infinite-dimensional Hilbert space, however, two arbitrary PVM's need not be unitarily related (e.g., for quadrature and photon-number measurements) and we have to restrict ourselves to a set of unitarily related PVM's* $\{\hat{\pi}_j(\cdot|y) = \hat{u}(y)\hat{\Pi}_j(\cdot)\hat{u}(y)^\dagger : y \in \prod_{k=1}^{j-1}\Omega_k\}$. *It's not that bad a restriction—for example, we know from Chap. 8 that optical homodyne detection is implemented with a local oscillator and square-law detectors, so the local oscillator can be regarded as an ancilla and a real homodyne detector is unitarily related to photon counting after-all. For the homodyne detector to implement a quadrature measurement exactly, the local oscillator needs to be infinitely strong, but we don't have that in reality.*

(2) With n such maps, we use Eq. (B.123) to defer each partial trace repeatedly to obtain

$$\mathcal{F}_n(x_n|y_n)\ldots\mathcal{F}_1(x_1)\hat{\rho} = \mathrm{tr}_{D_n}\ldots\mathrm{tr}_{D_1}\left(\hat{W}_1\hat{\rho}\hat{W}_1^\dagger\right), \tag{G.81}$$

$$\hat{W}_n \equiv \left[\hat{I}_n \otimes \hat{\Pi}_n(x_n)\right]\hat{U}_n(y_n)\,|\psi_n\rangle, \tag{G.82}$$

$$\hat{W}_j \equiv \left[\hat{W}_{j+1} \otimes \hat{\Pi}_j(x_j)\right]\hat{U}_j(y_j)\,|\psi_j\rangle, \quad j = n-1,\ldots,1, \tag{G.83}$$

where

$$\hat{W}_n : \mathcal{H}_{n-1} \to \mathcal{H}_{n-1}\otimes\mathcal{H}_{B_n} \sim \mathcal{H}_n \otimes \mathcal{H}_{D_n}, \qquad \hat{W}_j : \mathcal{H}_{j-1} \to \mathcal{H}_n \otimes \mathcal{H}_{D_n}\otimes\cdots\otimes\mathcal{H}_{D_j}. \tag{G.84}$$

(3) Key step: we repeatedly defer each $\hat{\Pi}_j$ to a later time using the identity

$$\boxed{\hat{A}(x)\otimes\hat{\Pi}(x) = \left[\hat{I}\otimes\hat{\Pi}(x)\right]\sum_z \hat{A}(z)\otimes\hat{\Pi}(z),} \tag{G.85}$$

which comes from $\hat{\Pi}(x)\hat{\Pi}(z) = \hat{\Pi}(x)\delta_{xz}$ for a PVM with discrete outcomes x and z. We obtain

$$\hat{W}_1 = \left[\hat{I}_n \otimes \hat{\Pi}_n(x_n)\otimes\cdots\otimes\hat{\Pi}_1(x_1)\right]\hat{w}_n\ldots\hat{w}_1, \tag{G.86}$$

$$\hat{w}_j \equiv \sum_{z_{j-1},\ldots,z_1} \hat{U}_j(z_{j-1},\ldots,z_1)\,|\psi_j\rangle \otimes \hat{\Pi}_{j-1}(z_{j-1})\otimes\cdots\otimes\hat{\Pi}_1(z_1), \tag{G.87}$$

where

$$\hat{w}_1 : \mathcal{H}_0 \to \mathcal{H}_0\otimes\mathcal{H}_{B_1} \sim \mathcal{H}_1\otimes\mathcal{H}_{D_1}, \tag{G.88}$$

$$\hat{w}_j : \mathcal{H}_{j-1}\otimes\mathcal{H}_{D_{j-1}}\otimes\ldots\mathcal{H}_{D_1} \to \mathcal{H}_j\otimes\mathcal{H}_{D_j}\otimes\ldots\mathcal{H}_{D_1}, \quad j = 2,\ldots,n. \tag{G.89}$$

(4) The final result is

$$\boxed{\mathcal{F}_n(x_n|y_n)\dots\mathcal{F}_1(x_1)\hat{\rho} = \mathrm{tr}_{D_n}\dots\mathrm{tr}_{D_1}\left\{\left[\hat{I}_n\otimes\hat{\Pi}_n(x_n)\otimes\cdots\otimes\hat{\Pi}_1(x_1)\right]\hat{\tau}_n\right\},} \tag{G.90}$$

$$\boxed{\hat{\tau}_j = \hat{V}_j(\hat{\tau}_{j-1}\otimes\hat{\sigma}_j)\hat{V}_j^\dagger,} \quad j=1,\dots,n, \quad \hat{\tau}_0=\hat{\rho}, \tag{G.91}$$

$$\boxed{\hat{V}_j \equiv \sum_{z_{j-1},\dots,z_1}\hat{U}_j(z_{j-1},\dots,z_1)\otimes\hat{\Pi}_{j-1}(z_{j-1})\otimes\cdots\otimes\hat{\Pi}_1(z_1),} \tag{G.92}$$

where each $\hat{\tau}_{j-1}$ is on $\mathcal{H}_0\otimes\mathcal{H}_{B_1}\otimes\cdots\otimes\mathcal{H}_{B_{j-1}}$, $\hat{\tau}_{j-1}\otimes\hat{\sigma}_j$ is on $\mathcal{H}_0\otimes\mathcal{H}_{B_1}\otimes\cdots\otimes\mathcal{H}_{B_j}$, $\hat{V}_j$ is on

$$\mathcal{H}_0\otimes\mathcal{H}_{B_1}\otimes\cdots\otimes\mathcal{H}_{B_j}\sim\mathcal{H}_j\otimes\mathcal{H}_{D_j}\otimes\cdots\otimes\mathcal{H}_{D_1}, \tag{G.93}$$

and Eq. (G.92) applies to the latter order. The dynamics is now fully unitary, as modeled by the controlled unitaries $\{\hat{V}_j\}$, while all the measurements have been deferred to the final time, as modeled by $\hat{I}_n\otimes\hat{\Pi}_n(x_n)\otimes\cdots\otimes\hat{\Pi}_1(x_1)$.

(5) The principle can be verified by observing that the two models give the same probability distribution:

$$P_{X_n,\dots,X_1}(x_n,\dots,x_1) = \mathrm{tr}\left[\mathcal{F}_n(x_n|y_n)\dots\mathcal{F}_1(x_1)\hat{\rho}\right] = \mathrm{tr}\left\{\left[\hat{I}_n\otimes\hat{\Pi}_n(x_n)\otimes\cdots\otimes\hat{\Pi}_1(x_1)\right]\hat{\tau}_n\right\}. \tag{G.94}$$

Exercise G.9. Prove that $\hat{V}_j$ is unitary and $\hat{I}_n\otimes\hat{\Pi}_n(x_n)\otimes\cdots\otimes\hat{\Pi}_1(x_1)$ is a PVM.

G.11. Church of the larger Hilbert space

We stress that open quantum system theory does not modify quantum physics in any way; the former merely introduces a suite of mathematical tools to describe the latter more succinctly when we partition the universe—somewhat arbitrarily and artificially—into a system of interest and some ancillas. In fact, for some problems, it may be easier and more general to stick to ordinary quantum mechanics in terms of pure states, unitaries, and projective measurements. The price to pay is that the Hilbert space needs to be large enough to accommodate all the system and ancillary degrees of freedom, so brute-force simulations may be challenging.

The fact that ordinary quantum mechanics, with a sufficiently large Hilbert space, can be used to model open quantum systems is sometimes called "the church of the larger Hilbert space." The principle of deferred measurement, in particular, underlies the Everett interpretation of quantum mechanics, which says that any observer can be modeled as a quantum ancilla and the measurement modeled as a quantum interaction between the system and the ancilla, so that Born's rule is unnecessary—an illusion.

Despite this radical viewpoint, Born's rule remains very convenient. In Sec. G.10, we still have to use Born's rule for the final PVM to verify the principle of deferred measurement. Everett's interpretation also doesn't explain why Born's rule works so well in practice. Born's rule is an oddball in quantum foundations that awaits a more satisfying explanation.

APPENDIX H

Statistics*

H.1. Introduction

The goal of any experiment, especially in sensing and imaging, is to infer unknowns from noisy data. The measurement is not the end of the story, and the data need to be further processed. The accuracy of our inference thus depends not only on the quality of the measurement but also the method of the processing. To devise a performance metric that accounts for both, the signal-to-noise ratio (SNR) we used in previous chapters turns out to be inadequate. From this chapter and the next few, we introduce the necessary statistics so that we have more holistic ways of assessing the performance of an experiment, including the data processing.

Remark H.1. *We can make a distinction between probability and statistics as two disciplines:*

- *Probability theory, as outlined in Appendix C, assumes **one probability measure** and studies its various properties, such as the probability of an event and the expected values of random variables.*
- *Statistics (in the sense of a discipline studied by statisticians) assumes **a set of probability measures** called the statistical model, all with the same sample space Ω and event space E. An **observation** is assumed to be a random variable that comes from one of the probability measures, and our goal is to learn certain properties of the model from the observation.*

In statistics, the terms inference, decision, detection, hypothesis testing, and estimation are all fancy words for the act of guessing in various contexts.

H.2. Statistical model

To define a statistical model, we introduce a new variable called the **parameter** $\theta \in \Theta$ to label a set of probability measures, where Θ is called the **parameter space**. Then a statistical model is defined as a set of probability measures

$$\{P_\theta : \theta \in \Theta\}, \tag{H.1}$$

where each $P_\theta : E \to [0, 1]$ for a given θ is a candidate measure for our observation. For most problems, there exists a θ-independent reference measure σ that dominates all measures in the model, and we call the Radon-Nikodym derivative (see Sec. C.9)

$$f_\theta(x) \equiv \frac{dP_\theta}{d\sigma}(x) \tag{H.2}$$

the probability density.

(1) If the observation is discrete, then we take σ to be the counting measure so that

$$\boxed{d\sigma(x) = 1,} \qquad \boxed{dP_\theta(x) = f_\theta(x) = P_\theta(x),} \tag{H.3}$$

and the expectation of a random variable $g(x)$ conditioned on θ becomes

$$\boxed{\mathbb{E}_\theta(g) \equiv \int g(x) dP_\theta(x) = \sum_x g(x) P_\theta(x).} \tag{H.4}$$

(2) If $\Omega \subseteq \mathbb{R}^n$, we take σ to be the Lebesgue measure so that $f_\theta(x)$ is the conventional probability density, and we write

$$\boxed{d\sigma(x) = d^n x,} \qquad \boxed{dP_\theta(x) = f_\theta(x) d^n x,} \qquad \boxed{\mathbb{E}_\theta(g) = \int g(x) f_\theta(x) d^n x.} \tag{H.5}$$

Remark H.2. *Beware that θ in P_θ or f_θ does not denote a random variable for a probability mass function or probability density, unlike the notation in Appendix C; here θ is an additional label of the measure.*

Two basic examples of a parameter space Θ:

(1) If Θ is discrete, e.g., $\Theta = \{0, 1, 2, \dots\}$, then the parameter is more commonly called a **hypothesis**, and the inference is commonly called **hypothesis testing**.

The simplest example is when there are only two elements in Θ, commonly denoted as $\Theta = \{0, 1\}$. Then there are only two probability measures P_0 and P_1 in the model, and the inference is called binary hypothesis testing or detection. $\theta = 0$ is commonly called the null hypothesis, and $\theta = 1$ is called the alternative hypothesis. Examples:

(a) Radar detection: The radar readings are the observations. $\theta = 0$ denotes the hypothesis that a target is absent, while $\theta = 1$ denotes the hypothesis that a target is present.

(b) Tumor detection: The X-ray images are the observations. $\theta = 0$ denotes the hypothesis that a tumor is absent, while $\theta = 1$ denotes the hypothesis that a tumor is present.

(c) Gravitational-wave detection: The data from our optical measurements are the observations. $\theta = 0$ denotes the hypothesis that no gravitational wave hits the detector, while $\theta = 1$ denotes the hypothesis that a gravitational wave is there.

Remark H.3. *Outside statistics, the words detection and detector refer to a generic measurement and a generic measurement device, e.g., homodyne detection and gravitational-wave detector, whereas detection in statistics means something more specific: the detection of a target in binary hypothesis testing.*

(2) If Θ is continuous, e.g., $\Theta = \mathbb{R}^p$ or a subset with non-empty interior, then $\theta \in \Theta$ is commonly called a parameter and Θ a parameter space. The inference is commonly called **parameter estimation**. Examples:

(a) Radar, X-ray: suppose that a target is present. We'd like to estimate its size and shape, which are modeled by real numbers.

(b) Gravitational-wave estimation: estimate the gravitational waveform as a function of time.

(c) Astronomy, microscopy, spectroscopy: estimate the positions, brightnesses, shapes, and intensity distributions of stars, particles, or spectral lines.

If Θ is multidimensional, e.g., $\Theta \subseteq \mathbb{R}^p$ with $p > 1$, then the task is sometimes called multiparameter estimation, as there are multiple components in each parameter θ. We model it by a vectoral θ.

(3) In practice, one may wish to perform both hypothesis testing and parameter estimation from one set of data, e.g., tumor detection and measurement from an X-ray image, in which case the task is called composite hypothesis testing.

H.3. Decision rule

Our next task is to model our guess of the parameter mathematically. Given an observation $x \in \Omega$, we model our guess by a function

$$\check{\theta} : \Omega \times \Omega' \to \Theta \tag{H.6}$$

called a **decision rule**, also called an **estimator** in parameter estimation. The decision may depend not only on the observation $x \in \Omega$ but also an independent **ancilla** random variable $y \in \Omega'$. When a decision rule involves such an ancilla, we say that the rule is randomized, otherwise it is deterministic. In other words, a deterministic rule will always give the same guess $\check{\theta}(x)$ for the same observation x, while a randomized rule $\check{\theta}(x, y)$ depends also on the random ancilla y so the guess may be different in each trial for the same observation x. We allow randomized rules because they may be advantageous in special cases, to hedge among a bunch of deterministic rules.

H.4. Loss function

To carry out the first step of quantifying the statistical performance, we define a **loss function** $l(\theta, \check{\theta})$ that quantifies the difference between the true parameter θ and our guess $\check{\theta}(x)$. Examples:

(1) For hypothesis testing, the **zero-one loss** is common:

$$l(\theta, \check{\theta}) = 1 - \delta_{\theta\check{\theta}} = \begin{cases} 0, & \check{\theta} = \theta, \\ 1, & \check{\theta} \neq \theta. \end{cases} \tag{H.7}$$

(2) For parameter estimation where $\theta \in \Theta \subseteq \mathbb{R}$ is a scalar parameter, the **square loss** is common:

$$l(\theta, \check{\theta}) = \big(\theta - \check{\theta}\big)^2. \tag{H.8}$$

(3) If Θ is a normed vector space, then we can use the norm to quantify the distance:

$$l(\theta, \check{\theta}) = \big\|\theta - \check{\theta}\big\|^2. \tag{H.9}$$

For example, if Θ is an inner product space, we can pick

$$\big\|\theta - \check{\theta}\big\|^2 = \big\langle \theta - \check{\theta}, \theta - \check{\theta} \big\rangle \tag{H.10}$$

in terms of the inner product. In particular, the standard l^2 norm for $\mathbb{R}^p$ is

$$\big\|\theta - \check{\theta}\big\|^2 = \sum_{j=1}^{p} \big(\theta_j - \check{\theta}_j\big)^2, \tag{H.11}$$

or one may pick

$$\big\|\theta - \check{\theta}\big\|^2 = \sum_{j,k} \big(\theta_j - \check{\theta}_j\big) G_{jk} \big(\theta_k - \check{\theta}_k\big), \tag{H.12}$$

where G is a positive-definite matrix.

Side note. *In some areas of machine learning, people prefer to define a reward function instead. Just put a minus sign on a loss function to obtain a reward function, or in general apply any decreasing function to convert a loss to a reward and vice versa.*

H.5. Errors of a decision

Often we do not know the ground truth θ. After we have made an observation (x, y) and a decision $\check{\theta}(x, y)$, we need to quantify the uncertainty about the particular decision. In other words, we would like to put an **error bar** on our experimental result. The concepts of p-value, confidence interval, Bayesian posterior errors, bootstrap, etc., are all invented for that purpose, but we won't go into the details of them; see, for example, Ref. [52].

H.6. Errors of a rule

The decision rule $\check{\theta}(x, y)$ is a function of the observation x and the ancilla y, which are independent random variables sampled from the product probability measure (see Sec. C.3)

$$\mathcal{P}_\theta \equiv P_\theta \otimes P'. \tag{H.13}$$

With random x and y, $\check{\theta}$ and $l(\check{\theta}, \theta)$ become random variables. To study the average loss of a rule over many trials, we consider the expected loss:

$$R(\theta, \check{\theta}) \equiv \mathbb{E}_\theta \big[l(\theta, \check{\theta})\big] = \int l(\theta, \check{\theta}(x, y)) d\mathcal{P}_\theta(x, y), \tag{H.14}$$

where $\mathbb{E}_\theta$ denotes the expectation with respect to $\mathcal{P}_\theta$ for a fixed θ. We will simply call this R **the error**. It is sometimes called the risk function in the literature. The error $R(\theta, \check{\theta})$ is a function of the true parameter θ and also the rule $\check{\theta}$, but it no longer depends on the observation x and the ancilla y. For example,

(1) if we use the zero-one loss for binary hypothesis testing, then

$$R(0,\check{\theta}) = \mathbb{E}_0\left(1-\delta_{\check{\theta}0}\right) = \int_{(x,y):\check{\theta}(x,y)=1} d\mathcal{P}_0(x,y) = \mathcal{P}_0\big[\check{\theta}=1\big] \tag{H.15}$$

is the probability of a false alarm, also called a false positive or a type-I error. In this case, $\theta = 0$ is the truth, while $\{(x,y) : \check{\theta}(x,y) = 1\}$ is the set of (augmented) observations that make us decide on the alternative hypothesis. Similarly,

$$R(1,\check{\theta}) = \mathbb{E}_1\left(1-\delta_{\check{\theta}1}\right) = \int_{(x,y):\check{\theta}(x,y)=0} d\mathcal{P}_1(x,y) = \mathcal{P}_1\big[\check{\theta}=0\big] \tag{H.16}$$

is the probability of a miss, also called a false negative or a type-II error. In this case, $\theta = 1$ is the truth, while $\{(x,y) : \check{\theta}(x,y) = 0\}$ is the set of observations that make us decide on the null hypothesis.

(2) For scalar parameter estimation, the **mean-square error** is

$$R(\theta,\check{\theta}) = \int \big[\theta - \check{\theta}(x,y)\big]^2 d\mathcal{P}_\theta(x,y). \tag{H.17}$$

The error $R(\theta,\check{\theta})$ is a function of the parameter $\theta \in \Theta$ and may be difficult to study if the parameter space Θ is large. To further simplify it, we define the **average error**

$$R_\pi(\check{\theta}) \equiv \int R(\theta,\check{\theta}) d\pi(\theta) \tag{H.18}$$

with respect to a **prior** probability measure π on (Θ, G) for the parameter, where G is an event space for Θ, and the **worst-case error**:

$$\max_{\theta\in\Theta} R(\theta,\check{\theta}). \tag{H.19}$$

These two errors are summaries about $R(\theta,\check{\theta})$—they are now functions of the decision rule $\check{\theta}$ only. They obey the inequality

$$\max_{\theta\in\Theta} R(\theta,\check{\theta}) \geq R_\pi(\check{\theta}) \tag{H.20}$$

for any prior π. Fig. H.1 illustrates the three errors.

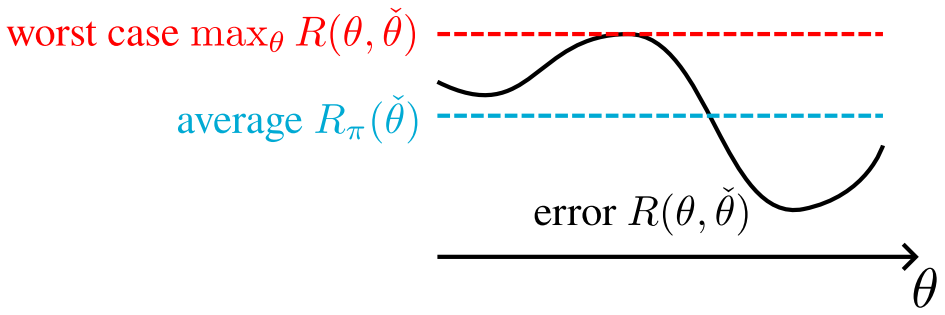

FIGURE H.1. Given a decision rule $\check{\theta}$, $R(\theta,\check{\theta})$ is the error as a function of the parameter θ, $R_\pi(\check{\theta})$ is the average with respect to a prior measure π for θ, and $\max_\theta R(\theta,\check{\theta})$ is the worst-case error.

Side note. *For rigor, mathematicians often use* inf *and* sup *instead of* min *and* max*, since the latter may not exist for certain sets, but for practitioners it is splitting infinitesimal hairs. We write* min *and* max *exclusively in this book.*

H.7. Errors of an experiment

A nice fact about the average error $R_\pi(\check{\theta})$ and the worst-case error $\max_\theta R(\theta, \check{\theta})$ is that there exists a strategy that minimizes each. The decision rule $\check{\theta}$ that minimizes the average error $R_\pi(\check{\theta})$ is a deterministic rule called **Bayesian** or **Bayes**, given by

$$\check{\theta}_{\text{Bayes}}(x) = \arg\min_{\phi\in\Theta} \int l(\theta, \phi) dQ_x(\theta), \tag{H.21}$$

where Q_x is the posterior measure on the parameter space (Θ, G) conditioned on the observation x, determined by the Bayes theorem

$$Q_x(A) = \frac{\int_{\theta\in A} f_\theta(x) d\pi(\theta)}{\int_{\theta\in\Theta} f_\theta(x) d\pi(\theta)}, \quad A \in G, \tag{H.22}$$

and $\int l(\theta, \phi) dQ_x(\theta)$ is the posterior error. For example, for the square loss, the Bayes rule is the conditional expectation

$$\check{\theta}_{\text{Bayes}}(x) = \int \theta dQ_x(\theta). \tag{H.23}$$

In general, the minimum average error

$$R_{\text{Bayes}}(\pi) \equiv \min_{\check{\theta}} R_\pi(\check{\theta}) = R_\pi(\check{\theta}_{\text{Bayes}}) \tag{H.24}$$

achieved by the Bayes rule is called the **Bayes error**.

The rule $\check{\theta}_{\text{minimax}}$ that minimizes the worst-case error $\max_{\theta\in\Theta} R(\theta, \check{\theta})$ is called **minimax**, such that the minimum worst-case error

$$R_{\text{minimax}} \equiv \min_{\check{\theta}} \max_{\theta\in\Theta} R(\theta, \check{\theta}) = \max_{\theta\in\Theta} R(\theta, \check{\theta}_{\text{minimax}}) \tag{H.25}$$

is called the **minimax error**. Eq. (H.20) leads to

$$\boxed{R_{\text{minimax}} \geq R_\pi(\check{\theta}_{\text{minimax}}) \geq \min_{\check{\theta}} R_\pi(\check{\theta}) = R_{\text{Bayes}}(\pi).} \tag{H.26}$$

Under certain conditions, the two errors $R_{\text{Bayes}}(\pi)$ and R_{minimax} can coincide for a certain prior π called the least favorable prior. Then the Bayes rule for the least favorable prior is the same as the minimax rule. See, for example, Ref. [53] for further details.

Side note. *The worst-case error and the minimax rule are much more difficult to study mathematically but are favoured by statisticians who don't like to assume a prior, as well as computer scientists.*

Errors such as R_{Bayes} and R_{minimax} no longer depend on the decision rule, so they are figures about an experiment assuming that optimal data processing can be performed. These errors can be used as benchmarks for quantifying and comparing the performances of measurement devices for sensing and imaging. They are far more meaningful than the SNR we used in previous chapters, because the errors have taken the data processing into account and represent the *final-stage* performance of a measurement task.

While it is generally true that, assuming optimal processing for a given device, the higher the SNR, the lower the errors, the specific relations between the SNR and the errors can be quite nontrivial and depend on the statistical model. For different devices with different noise types, e.g., photon counting versus homodyne detection, their SNRs can't tell us precisely which one has lower errors after data processing, and we should use the errors as the more conclusive benchmarks.

H.8. Side note: caveats and virtues of statistics

Statistics is as challenging as it is important. Some key challenges:

(1) **System identification**: An accurate and useful statistical model requires a careful calibration of the experiment.
(2) **Curse of dimensionality**: A huge number of unknown parameters may be needed for an accurate statistical model. In other words, the parameter space Θ for a statistical model may have a huge number of dimensions. For example, the space of candidate gravitational waves is a function space, often modeled as a space with very high dimensions or even an infinite-dimensional space.
(3) Even if one has a decent model, the optimal rules and quantities may be difficult to compute. The difficulties are on many levels:
    (a) **Theoretical complexity**: While the fundamental decision theory is in place, there may not be closed-form or accurate solutions to the optimal rules and quantities.
    (b) **Human skill**: Even if good solutions exist in the literature, a practitioner may find the theory challenging to digest or they may harbor misconceptions to use it correctly.
    (c) **Human effort**: Even if a practitioner understands the theory (or finds a collaborator who does), the solutions may require a lot of effort to derive, or the computer code may require a lot of effort to write.
    (d) **Computational complexity**: Even if the code can be written, it may require a lot of computational resources to run.
(4) **Spherical cows**: If we dumb down our statistical model to make the theory easier, we run the risk of having a naive "spherical-cow" model of the reality (https://en.wikipedia.org/wiki/Spherical_cow). This is a major criticism of the traditional "model-based" approach in statistics [54].

    A famous aphorism is "All models are wrong, but some are useful" (https://en.wikipedia.org/wiki/All_models_are_wrong).

A major recent trend in data processing is, of course, "machine learning" and neural networks, which enable one to skip the statistical model and arrive directly at a decision rule by training with datasets. While they solve many of the aforementioned challenges, model-based statistics is still valuable for our purpose:

(1) **Decent physical models**: Compared to other disciplines such as social sciences, a good news for physics and engineering is that we often know our physical laws and devices pretty well, and simple statistical models such as Gaussian or Poisson are decent.
(2) **Experimental design**: The performance of any machine-learning technique for an experiment is difficult to assess until one runs it with some data, requiring a lot of time and effort. Without a simpler theory to guide us, it becomes difficult to design or modify an experiment to optimize or improve the end-stage performance.
(3) **Fundamental limits**: Even if one uses machine-learning techniques, theoretical statistics can still inform us the fundamental limits of large classes of data-processing techniques, in the same manner as the laws of thermodynamics.

With all the virtues and caveats of statistics in mind, we proceed with simple statistical problems in the next few chapters.

APPENDIX I

Binary Hypothesis Testing*

The simplest problem in statistics is binary hypothesis testing with parameter space $\Theta = \{0, 1\}$ and only two candidate probability measures P_0 and P_1 for the observation. To pick a decision rule, there are two common rules used in statistics: the Neyman-Pearson rule and the Bayes rule.

I.1. Neyman-Pearson rule

The rule calls for the false-alarm probability to be restricted below a tolerance level α and the miss probability to be minimized. In other words, the rule can be expressed as

$$\check{\theta}_{\text{NP}} \equiv \underset{\check{\theta}:\mathcal{P}_0[\check{\theta}=1]\leq\alpha}{\arg\min}\ \mathcal{P}_1[\check{\theta}=0]. \tag{I.1}$$

We call the resulting miss probability

$$R_{\text{NP}}(\alpha) \equiv \min_{\check{\theta}:\mathcal{P}_0[\check{\theta}=1]\leq\alpha} \mathcal{P}_1[\check{\theta}=0] \tag{I.2}$$

the Neyman-Pearson error. It can be shown that the Neyman-Pearson rule can be implemented by the so-called **likelihood-ratio test** [55, 56]. It is in terms of the **likelihood ratio**, a special case of the Radon-Nikodym derivative introduced in Sec. C.9:

$$\Lambda(x) \equiv \frac{dP_1}{dP_0}(x) = \frac{f_1(x)}{f_0(x)}. \tag{I.3}$$

In terms of the likelihood ratio, the likelihood-ratio test is the decision rule

$$\check{\theta}(x, y) = \begin{cases} 0, & \Lambda(x) < T(y), \\ 1, & \Lambda(x) \geq T(y), \end{cases} \tag{I.4}$$

where T is the test threshold, which may depend on the ancilla y.

The likelihood-ratio test illustrates the trade-off in minimizing the two errors $\mathcal{P}_0[\Lambda \geq T]$ and $\mathcal{P}_1[\Lambda < T]$. Raising the threshold T would decrease the false-alarm probability $\mathcal{P}_0[\Lambda \geq T]$ but increase the miss probability $\mathcal{P}_1[\Lambda < T]$, while lowering the threshold would do the opposite. It therefore makes sense that the optimal choice of T should make the false-alarm probability

$$\mathcal{P}_0[\check{\theta} = 1] = \mathcal{P}_0[\Lambda \geq T] = \alpha \tag{I.5}$$

hit the tolerance level α. For a given α, a randomized threshold T may be necessary if the observation and thus Λ are discrete.

I.2. Bayes rule

The Bayes rule is easier in many ways, as long as the prior probabilities π_0 and $\pi_1 = 1 - \pi_0$ are given for the two hypotheses. Here we seek to minimize the average error under the zero-one loss:

$$R_\pi(\check{\theta}) = \pi_0 \mathcal{P}_0[\check{\theta} = 1] + \pi_1 \mathcal{P}_1[\check{\theta} = 0], \tag{I.6}$$

which is a weighted average of the false-alarm probability and the miss probability. It has the operational meaning of the average error probability, since it is the probability of making any of the two types of errors. The Bayes rule given by Eq. (H.21) can be framed as a likelihood-ratio test with the threshold

$$T = \frac{\pi_0}{\pi_1}. \tag{I.7}$$

This fixed threshold is much more convenient to use in practice than the Neyman-Pearson rule according to Eq. (I.5), which may be quite hard to solve because $\mathcal{P}_0[\Lambda \geq T]$ as a function of T is often difficult to compute and then we need to invert it to obtain the desired T.

The resulting Bayes error has the nice formula [57, 58]

$$\boxed{R_{\text{Bayes}}(\pi) = \frac{1}{2} - K(\pi_0 P_0, \pi_1 P_1),} \tag{I.8}$$

where

$$\boxed{K(\pi_0 P_0, \pi_1 P_1) \equiv \sup_{A \in E} |\pi_0 P_0(A) - \pi_1 P_1(A)| = \frac{1}{2} \int |\pi_0 f_0(x) - \pi_1 f_1(x)| d\sigma(x)} \tag{I.9}$$

is called the **Kolmogorov distance** between two measures. K quantifies the distinguishability between the two hypotheses, so that the higher the K, the lower the error R_{Bayes}.

Side note. *The minimax rule seems far less commonly used in binary hypothesis testing; the Neyman-Pearson rule is standard if one doesn't like Bayes.*

For further details about binary hypothesis testing, see, for example, Refs. [55, 56].

I.3. Chernoff upper bounds

The Neyman-Pearson error R_{NP} given by Eq. (I.2) and the Bayes error R_{Bayes} given by Eq. (I.8) are useful figures about an experiment, but they are often very difficult to compute analytically or even numerically. Statisticians often resort to bounds on the errors and asymptotics to get a rough idea about them.

Assume the likelihood-ratio test with a deterministic threshold $0 < T < \infty$. Let

$$t \equiv \ln T \in \mathbb{R}, \tag{I.10}$$

which is the threshold if the likelihood-ratio test is in terms of the log likelihood ratio $\ln \Lambda$. Chebyshev's inequality (sometimes called Markov's inequality https://en.wikipedia.org/wiki/Markov%27s_inequality) yields

$$P_0[\Lambda \geq T] \leq T^{-s}\, \mathbb{E}_0\left(\Lambda^s\right) = \exp\left[-st + \mu(s)\right] \quad \forall s \geq 0, \tag{I.11}$$

$$P_1[\Lambda < T] \leq T^{1-s}\, \mathbb{E}_1\left(\Lambda^{s-1}\right) = \exp\left[(1-s)t + \mu(s)\right] \quad \forall s \leq 1, \tag{I.12}$$

where we call

$$\boxed{\mu(s) \equiv \ln \mathbb{E}_0\left(\Lambda^s\right) = \ln \mathbb{E}_1\left(\Lambda^{s-1}\right) = \ln \int f_1(x)^s f_0(x)^{1-s} d\sigma(x)} \tag{I.13}$$

the Chebyshev exponent. $\mu(s)$ is often much easier to compute analytically than the errors.

To obtain the tightest upper bounds, we set

$$s_{t0} \equiv \arg\max_{s \geq 0} \left[st - \mu(s)\right] \tag{I.14}$$

for the first bound in Eq. (I.11) and

$$s_{t1} \equiv \arg\max_{s \leq 1} \left[-(1-s)t - \mu(s)\right] \tag{I.15}$$

for the second bound in Eq. (I.12). Notice that the local extrema of both problems occur at $\dot{\mu}(s) = t$. Furthermore, notice the following properties of the Chebyshev exponent $\mu(s)$ when $P_0 \neq P_1$ [59]:

(1) $\mu(s)$ is strictly convex for $s \in \mathbb{R}$, i.e., $\ddot{\mu}(s) > 0$. This is because $\ln$ is strictly increasing and

$$\frac{\partial^2}{\partial s^2}\,\mathbb{E}_0(\Lambda^s) = \mathbb{E}_0\left[(\ln\Lambda)^2 e^{s\ln\Lambda}\right] > 0 \tag{I.16}$$

as long as $P_0 \neq P_1$, such that $\mathbb{E}_0(\Lambda^s)$ is strictly convex. It follows that $\dot{\mu}(s)$ is strictly increasing, and we can define

$$\nu(t) \equiv \max_{s\in\mathbb{R}}\left[st - \mu(s)\right] = s_t t - \mu(s_t), \quad \text{where } s_t \text{ satisfies } \dot{\mu}(s_t) = t \tag{I.17}$$

as the Legendre transform of $\mu(s)$ (https://en.wikipedia.org/wiki/Legendre_transformation). By the basic property of the Legendre transform, $\nu(t)$ is also strictly convex for all $t \in \mathbb{R}$ ($\ddot{\nu}(t) > 0$) and $\dot{\nu}(t)$ is strictly increasing.

(2) Define

$$\boxed{D(P_0\|P_1) \equiv \int \left[\ln\frac{dP_0}{dP_1}(x)\right] dP_0(x)} \tag{I.18}$$

as the **relative entropy**, also called the Kullback-Leibler (KL) divergence. Then

$$\dot{\mu}(0) = \mathbb{E}_0(\ln\Lambda) = -D(P_0\|P_1), \qquad \dot{\mu}(1) = \mathbb{E}_1(\ln\Lambda) = D(P_1\|P_0), \tag{I.19}$$

which are the expected values of the log likelihood ratio under the two hypotheses. Since $D = 0$ if and only if the two measures are equal and $D > 0$ otherwise, $\dot{\mu}(0) < 0$ and $\dot{\mu}(1) > 0$ as long as $P_0 \neq P_1$.

(3) With the strict convexity of $\mu(s)$, $\dot{\mu}(s)$ must be strictly increasing, meaning that

$$\dot{\mu}(s) < \dot{\mu}(0) \text{ for } s < 0, \qquad \dot{\mu}(s) > \dot{\mu}(1) \text{ for } s > 1. \tag{I.20}$$

All these facts imply that, as long as $P_0 \neq P_1$ and the threshold $t = \ln T$ is in the interval

$$-D(P_0\|P_1) = \dot{\mu}(0) = \mathbb{E}_0(\ln\Lambda) < t < \mathbb{E}_1(\ln\Lambda) = \dot{\mu}(1) = D(P_1\|P_0), \tag{I.21}$$

there is one and only one solution to $\dot{\mu}(s) = t$ for $s \in \mathbb{R}$ and the solution must occur inside the interval $0 < s < 1$. It follows that s_{t0} and s_{t1} given by Eqs. (I.14) and (I.15) coincide in the interval $(0, 1)$ and we can write

$$\boxed{P_0[\Lambda \geq T] = P_0[\ln\Lambda \geq t] \leq \exp\left[-\nu(t)\right],} \tag{I.22}$$

$$\boxed{P_1[\Lambda < T] = P_1[\ln\Lambda < t] \leq \exp\left[-\nu(t) + t\right],} \tag{I.23}$$

$$\nu(t) = s_t t - \mu(s_t), \quad \text{where } s_t \text{ satisfies } \dot{\mu}(s_t) = t, \quad 0 < s_t < 1. \tag{I.24}$$

The first inequality is an upper bound on the right tail area of the probability density of the log likelihood ratio $\lambda \equiv \ln\Lambda$ for $\lambda \in [t, \infty)$, $t > \mathbb{E}_0(\ln\Lambda)$, and $\theta = 0$, while the second inequality is an upper bound on the left tail area of the probability density for $\lambda \in (-\infty, t)$, $t < \mathbb{E}_1(\ln\Lambda)$, and $\theta = 1$, as depicted in Fig. I.1. If the threshold t is outside the interval $(\mathbb{E}_0(\ln\Lambda), \mathbb{E}_1(\ln\Lambda))$ bounded by the means, one of the tail areas would be quite large, prompting a redesign of t or the experiment.

Within the interval $s \in [0, 1]$, we can say more about the Chebyshev exponent $\mu(s)$ and its Legendre transform $\nu(t)$:

$$s = 0: \qquad \mu(0) = 0, \qquad t = \dot{\mu}(0) = \mathbb{E}_0\left(\ln\Lambda\right) = -D(P_0\|P_1) \equiv t_0, \tag{I.25}$$

$$\nu(t_0) = 0, \qquad \nu(t_0) - t_0 = D(P_0\|P_1), \tag{I.26}$$

$$s = 1: \qquad \mu(1) = 0, \qquad t = \dot{\mu}(1) = \mathbb{E}_1\left(\ln\Lambda\right) = D(P_1\|P_0) \equiv t_1, \tag{I.27}$$

$$\nu(t_1) = D(P_1\|P_0), \qquad \nu(t_1) - t_1 = 0. \tag{I.28}$$

$$0 < s < 1: \qquad \mu(s) < 0, \qquad (\text{Jensen's } \mathbb{E}_0(\Lambda^s) \leq [\mathbb{E}_0(\Lambda)]^s = 1, \text{etc.}) \tag{I.29}$$

$$t_0 < t < t_1: \qquad 0 < \nu(t) < D(P_1\|P_0), \qquad (\nu(t_0) = 0, \dot{\nu}(t_0) = 0, \ddot{\nu}(t) > 0) \tag{I.30}$$

$$D(P_0\|P_1) > \nu(t) - t > 0. \qquad (\text{exchange } P_0 \text{ and } P_1) \tag{I.31}$$

Fig. I.2 summarizes these findings.

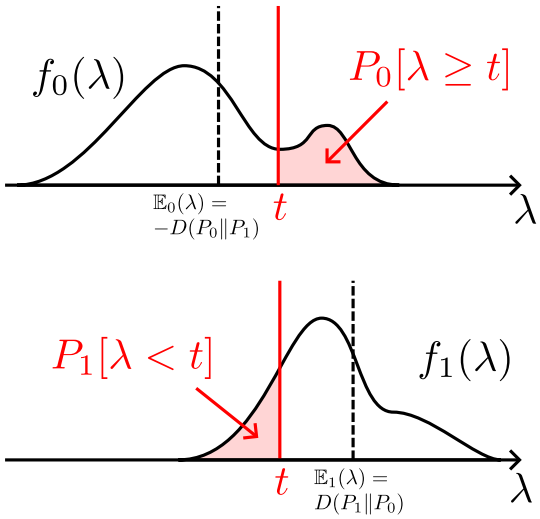

FIGURE I.1. $f_\theta(\lambda)$ is the probability density of the log-likelihood ratio $\lambda \equiv \ln \Lambda$ given the hypothesis $\theta = 0$ (top) or $\theta = 1$ (bottom); its mean is $\mathbb{E}_0(\lambda) = -D(P_0\|P_1)$ given $\theta = 0$ (top) or $\mathbb{E}_1(\lambda) = D(P_1\|P_0)$ given $\theta = 1$ (bottom). $P_0[\lambda \geq t]$ and $P_1[\lambda < t]$, the tail areas given a threshold t, are the error probabilities. If $t < \mathbb{E}_0(\lambda)$, the false-alarm probability $P_0[\lambda \geq t]$ would be very high; likewise for the miss probability $P_1[\lambda < t]$ if $t > \mathbb{E}_1(\lambda)$, so it is reasonable to assume that the threshold t stays in the interval $\mathbb{E}_0(\lambda) < t < \mathbb{E}_1(\lambda)$.

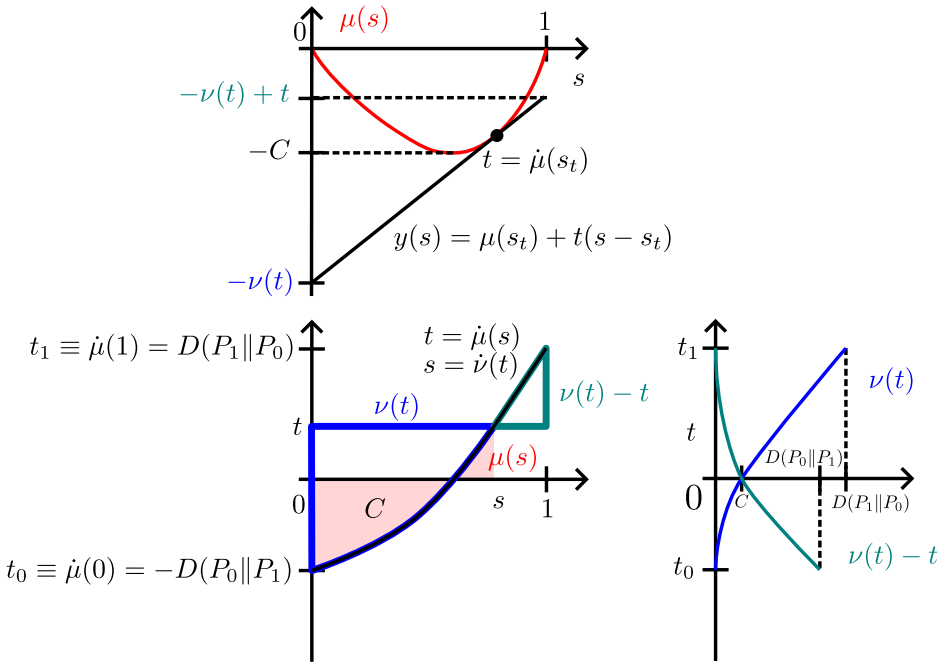

FIGURE I.2. Top: Chebyshev exponent $\mu(s)$ versus s for $s \in [0, 1]$. C is the Chernoff distance. The Legendre transform converts $\mu(s)$ to $\nu(t)$ via $s_t t - \mu(s_t)$ at $\dot{\mu}(s_t) = t$. Bottom left: Alternative picture of Legendre transform [60]. The curve is $t = \dot{\mu}(s)$ (vertical axis) versus s (horizontal axis). The same curve gives $s = \dot{\nu}(t)$ (horizontal axis) versus t (vertical axis). $\mu(s)$ is the signed area of the red region up to s. $\nu(t)$ is the absolute area enclosed by the blue boundary (blue lines and the curve). $\nu(t) - t$ is the absolute area enclosed by the green boundary (green lines and the curve). C is the absolute area of the red region up to $t = \dot{\mu}(s) = 0$. Bottom right: plot of $\nu(t)$ and $\nu(t) - t$ (horizontal axis) versus t (vertical axis).

For the Bayes rule with $T = \pi_1/\pi_0 = 1$ and $t = \ln T = 0$, in particular, Eq. (I.21) is satisfied and we obtain

$$\boxed{R_{\text{Bayes}}(1/2, 1/2) \le \frac{1}{2}\exp(-C),} \tag{I.32}$$

where

$$\boxed{C \equiv \nu(0) = \max_{0<s<1}[-\mu(s)]} \tag{I.33}$$

is called the **Chernoff distance**, which is another metric of distinguishability between two measures.

Eqs. (I.22), (I.23), and (I.32) are known as Chernoff bounds [55]. They serve as performance guarantees that the errors cannot exceed certain levels.

I.4. Large deviations

The Chernoff bounds are also tight in an asymptotic sense. Consider n i.i.d. (independent and identically distributed) observations $(x_1, \ldots, x_n) \in \Omega^n$ following the product measure (see Sec. C.3)

$$P_\theta^{(n)} = P_\theta^{\otimes n}. \tag{I.34}$$

Then the likelihood ratio becomes

$$\Lambda^{(n)}(x_1, \ldots, x_n) \equiv \frac{dP_1^{(n)}}{dP_0^{(n)}}(x_1, \ldots, x_n) = \Lambda(x_1)\ldots\Lambda(x_n), \tag{I.35}$$

where each $\Lambda(x_j)$ is the likelihood ratio for one observation x_j. Assume the likelihood-ratio test

$$\check{\theta}(x) = \begin{cases} 0, & \Lambda^{(n)} < T^{(n)}, \\ 1, & \Lambda^{(n)} \ge T^{(n)}, \end{cases} \tag{I.36}$$

and define

$$t \equiv \lim_{n\to\infty} \frac{1}{n}\ln T^{(n)} \tag{I.37}$$

as the growth rate of the threshold $T^{(n)}$, assumed to be finite. Then

$$T^{(n)} = \exp[nt + o(n)], \tag{I.38}$$

where $o(n)$ denotes terms asymptotically smaller than n, i.e.,

$$\lim_{n\to\infty} \frac{o(n)}{n} = 0. \tag{I.39}$$

For example, the Bayes rule has the fixed threshold $T^{(n)} = \pi_0/\pi_1$, so $t = 0$. The test inequalities can then be rewritten as

$$\frac{1}{n}\ln\Lambda^{(n)} = \frac{1}{n}\sum_{j=1}^{n}\ln\Lambda(x_j) \gtrless t + \frac{o(n)}{n}, \tag{I.40}$$

where the left-hand side is the sample mean of the log-likelihood ratio $\ln\Lambda$. Now assume

$$t > \mathbb{E}_0(\ln\Lambda) = -D(P_0\|P_1), \tag{I.41}$$

which is the same as the first inequality in Eq. (I.21). Then Cramér's theorem (https://en.wikipedia.org/wiki/Cram%C3%A9r%27s_theorem_(large_deviations)) gives the asymptotic decay rate of the false-alarm probability:

$$-\lim_{n\to\infty}\frac{1}{n}\ln P_0^{(n)}\left[\frac{1}{n}\ln\Lambda^{(n)} \ge t\right] = \max_{s\in\mathbb{R}}[st - \mu(s)], \tag{I.42}$$

where the $o(n)/n$ term can be thrown away in the limit and $\mu(s)$ is the Chebyshev exponent for one observation. A similar argument, assuming

$$t < \mathbb{E}_1(\ln \Lambda) = D(P_1 \| P_0), \tag{I.43}$$

which is the second inequality in Eq. (I.21), gives the asymptotic decay rate of the miss probability:

$$-\lim_{n\to\infty} \frac{1}{n} \ln P_1^{(n)} \left[\frac{1}{n} \ln \Lambda^{(n)} < t \right] = \max_{s\in\mathbb{R}} \left[-(1-s)t - \mu(s) \right]. \tag{I.44}$$

By the earlier arguments about the Legendre transform, as long as $P_0 \neq P_1$, we can write

$$-\lim_{n\to\infty} \frac{1}{n} \ln P_0^{(n)} \left[\frac{1}{n} \ln \Lambda^{(n)} \geq t \right] = \nu(t), \tag{I.45}$$

$$-\lim_{n\to\infty} \frac{1}{n} \ln P_1^{(n)} \left[\frac{1}{n} \ln \Lambda^{(n)} < t \right] = \nu(t) - t, \tag{I.46}$$

which are the same as the Chernoff bound exponents in Eqs. (I.22) and (I.23) for one observation.

If $t = 0$, the two decay rates coincide with the Chernoff distance C given by Eqs. (I.13) and (I.33). In particular,

$$-\lim_{n\to\infty} \frac{1}{n} \ln R_{\text{Bayes}}^{(n)}(\pi) = C, \tag{I.47}$$

where $R_{\text{Bayes}}^{(n)}(\pi)$ is the Bayes error in terms of $\{P_0^{(n)}, P_1^{(n)}\}$. It makes sense that the two decay rates should match under the Bayes rule, as increasing one would decrease the other, the asymptotic decay rate of the average error is the higher of the two, and the rule that minimizes the average error would make the two rates match.

I.5. Stein's lemma

Consider the Neyman-Pearson rule with n i.i.d. observations. Assume that a deterministic threshold $T^{(n)}$ satisfies the rule, so that

$$P_0^{(n)} \left[\Lambda^{(n)} \geq T^{(n)} \right] = \alpha. \tag{I.48}$$

Notice that this false-alarm probability stays constant and its decay rate is zero. Then Eq. (I.45) suggests that the threshold growth rate t satisfies $\nu(t) = 0$. It follows from Eqs. (I.26) and (I.46) that the asymptotic decay rate of the miss probability should be $\nu(t) - t = D(P_0 \| P_1)$, where D is the relative entropy for one observation given by Eq. (I.18). A more rigorous proof of this argument can be done to give

$$-\lim_{n\to\infty} \frac{1}{n} \ln R_{\text{NP}}^{(n)}(\alpha) = D(P_0 \| P_1), \tag{I.49}$$

where $R_{\text{NP}}^{(n)}$ denotes the Neyman-Pearson error given by Eq. (I.2) in terms of $\{P_0^{(n)}, P_1^{(n)}\}$. Equivalently, we can write

$$\boxed{R_{\text{NP}}^{(n)}(\alpha) = \exp\left[-nD(P_0 \| P_1) + o(n) \right].} \tag{I.50}$$

This result is called Stein's lemma.

Note that there is no limit on the absolute size of $\exp[o(n)]$, only that its exponent must vary sublinearly with n. Thus, Stein's lemma—and statements about asymptotic decay rates in general—are not at all precise about the absolute error for any finite n. Note also that $D(P_0 \| P_1)$ does not depend on the tolerance level α; only the $o(n)$ term depends on α.

I.6. Bayes error bounds

The Chernoff bounds are upper error bounds, and often we would like lower error bounds as well, which serve as fundamental limits to how low the errors can go. Here are some handy inequalities for the Bayes error [57, 58]:

$$\boxed{\pi_0\pi_1 e^{-2B} \le \frac{1}{2}\left(1-\sqrt{1-4\pi_0\pi_1 e^{-2B}}\right) \le R_{\text{Bayes}}(\pi) \le \sqrt{\pi_0\pi_1}e^{-B},} \tag{I.51}$$

where

$$\boxed{B \equiv -\mu(1/2) = -\ln\int\sqrt{f_0(x)f_1(x)}d\sigma(x)} \tag{I.52}$$

is called the **Bhattacharyya distance**. Defining two more distances related to the relative entropies as

$$D_{\min} \equiv \min\{D(P_0\|P_1), D(P_1\|P_0)\}, \qquad \tilde{D} \equiv \left[\frac{1}{D(P_0\|P_1)}+\frac{1}{D(P_1\|P_0)}\right]^{-1}, \tag{I.53}$$

which obey

$$\frac{1}{2}D_{\min} \le \tilde{D} \le D_{\min}, \qquad \left(\frac{1}{1/x+1/x} \le \frac{1}{1/x+1/y} \le \frac{1}{1/x} \text{ for } y \ge x > 0\right) \tag{I.54}$$

we obtain the following handy inequalities concerning $D_{\min}$, $\tilde{D}$, the Bhattacharyya distance B, the Chernoff distance C given by Eq. (I.33):

$$\boxed{B \le C \le 2B \le D_{\min},} \qquad \boxed{C \le \tilde{D}.} \tag{I.55}$$

The first inequality $B \le C$ comes from the defintions of B and C, the second $C \le 2B$ comes from combining Eqs. (I.47) and (I.51) for n i.i.d. observations, the third $2B \le D_{\min}$ comes from the theory of Rényi divergences [61], and the fourth $C \le \tilde{D}$ can be proved using the Legendre-transform theory in Sec. I.3 and is tighter than the bound $C \le D_{\min}$ [62].

Interesting observations:

(1) Eq. (I.55) means that B and C are within a factor of 2 of each other, as we can also write $C/2 \le B \le C$, while the relative entropies are somewhat higher. B is hence a decent substitute of C if the latter is too difficult to compute.

(2) $C \le D_{\min}$ can also be observed from Fig. I.2 and proved using the Legendre-transform theory there. It makes sense that C, the Bayes error decay rate, should be lower than $D(P_0\|P_1)$, the Neyman-Pearson error decay rate, since the Bayes rule minimizes the average error, requiring both decay rates to be low, while the Neyman-Pearson rule permits the false-alarm decay rate to stay constant, allowing the miss probability to decay faster.

With C being symmetric under the exchange of P_0 and P_1, $C \le D(P_1\|P_0)$ follows from the same argument.

(3) The tighter bound $C \le \tilde{D}$ can be proved as follows. Since $\ddot{\nu}(t) \ge 0$, $\dot{\nu}(t_a) \le \dot{\nu}(t_b)$ for $t_a \le t_b$. By the mean value theorem, there exist a $t_a \in [t_0, 0]$ and a $t_b \in [0, t_1]$ such that

$$\dot{\nu}(t_a) = \frac{\nu(0)-\nu(t_0)}{-t_0} \le \frac{\nu(t_1)-\nu(0)}{t_1} = \dot{\nu}(t_b), \qquad \frac{C}{D(P_0\|P_1)} \le \frac{D(P_1\|P_0)-C}{D(P_1\|P_0)}, \tag{I.56}$$

which results in $C \le \tilde{D}$.

Remark I.1. *Mathematicians have a stricter definition of distances and metrics (https://en.wikipedia.org/wiki/Metric_space). A Riemannian metric is another type of metric specific to differential geometry (https://en.wikipedia.org/wiki/Riemannian_manifold). We use the terms distance and metric loosely in this book and they may not satisfy the strict definitions.*

Side note. *There are a whole zoo of distances for probability measures; we've discussed only a few that have important operational meanings. More notable examples:*

(1) The Hellinger distance (https://en.wikipedia.org/wiki/Hellinger_distance) is related to the Bhattacharyya distance by

$$H \equiv \sqrt{1 - e^{-B}}. \tag{I.57}$$

The former is more common in statistics, while the latter is more common in engineering. They are, of course, equivalent concepts.

(2) The Rényi divergences are defined as [61]

$$D_s(P_0\|P_1) \equiv -\frac{\mu(1-s)}{1-s}, \quad s \in (0,1)\cup(1,\infty). \tag{I.58}$$

For $s = 0, 1,$ or ∞, D_s is defined by taking the limit $s \to 0, 1,$ or ∞. Then

$$B = \frac{1}{2}D_{1/2}(P_0\|P_1), \qquad D(P_0\|P_1) = D_1(P_0\|P_1). \tag{I.59}$$

$2B \le D$ comes from the fact that, given a pair of probability measures, D_s is an increasing function of s ($D_s \le D_{s'}$ for $s < s'$).

I.7. Properties of statistical distances

By virtue of the error bounds, statistical distances such as B, C, D are appealing alternatives to the exact errors, as the former are often easier to compute by hand or numerically. Their evaluation can be eased further by various special cases and more bounds.

I.7.1. n independent observations. Let $(x_1, \dots, x_n) \in \Omega_1 \times \cdots \times \Omega_n$ be independent observations following the product measure

$$P_\theta^{(n)} = P_{\theta,1} \otimes \cdots \otimes P_{\theta,n}, \tag{I.60}$$

where each $P_{\theta,j}$ is a probability measure on (Ω_j, E_j) and the individual measures $\{P_{\theta,j} : j = 1, \dots, m\}$ need not be the same. Let $\mu_j(s)$, B_j, C_j, $D(P_{0,j}\|P_{1,j})$ be the Chebyshev exponent, Bhattacharyya distance, Chernoff distance, and relative entropy with respect to $\{P_{0,j}, P_{1,j}\}$, respectively, and $\mu^{(n)}(s)$, $B^{(n)}$, $C^{(n)}$, and $D(P_0^{(n)}\|P_1^{(n)})$ be those with respect to $\{P_0^{(n)}, P_1^{(n)}\}$. Then

$$\mu^{(n)}(s) = \sum_{j=1}^n \mu_j(s), \qquad B^{(n)} = \sum_{j=1}^n B_j, \tag{I.61}$$

$$C^{(n)} = \max_{0\le s\le 1}\left[-\mu^{(n)}(s)\right] \le \sum_{j=1}^n C_j, \qquad D(P_0^{(n)}\|P_1^{(n)}) = \sum_{j=1}^n D(P_{0,j}\|P_{1,j}). \tag{I.62}$$

I.7.2. n i.i.d. observations. If the individual measures are identical with $P_{\theta,j} = P_\theta$, such that the observations are i.i.d. with $\mu_j(s) = \mu(s)$, $B_j = B$, and $C_j = C$, then

$$\boxed{\mu^{(n)}(s) = n\mu(s),} \qquad \boxed{B^{(n)} = nB,} \qquad \boxed{C^{(n)} = nC,} \qquad \boxed{D(P_0^{(n)}\|P_1^{(n)}) = nD(P_0\|P_1).} \tag{I.63}$$

I.7.3. Gaussian. Let the observation be the vectoral normal random variable $X \sim \mathcal{N}(m_\theta, \Sigma_\theta)$, wnere m_θ is an $n \times 1$ column vector and Σ_θ is an $n \times n$ covariance matrix. Then [57, 59]

$$\mu(s) = -\frac{1}{2}\left\{s(1-s)(m_1-m_0)^\top[s\Sigma_0 + (1-s)\Sigma_1]^{-1}(m_1-m_0) + \ln\frac{\det[s\Sigma_0 + (1-s)\Sigma_1]}{\det\left(\Sigma_0^s\Sigma_1^{1-s}\right)}\right\}, \tag{I.64}$$

$$B = \frac{1}{2}\left[\frac{1}{4}(m_1-m_0)^\top\left(\frac{\Sigma_0+\Sigma_1}{2}\right)^{-1}(m_1-m_0) + \ln\frac{\det[(\Sigma_0+\Sigma_1)/2]}{\det\sqrt{\Sigma_0\Sigma_1}}\right], \tag{I.65}$$

$$D(P_0\|P_1) = \frac{1}{2}\left[(m_1-m_0)^\top\Sigma_1^{-1}(m_1-m_0) + \operatorname{tr}(\Sigma_1\Sigma_0^{-1}) - \ln\det\left(\Sigma_1\Sigma_0^{-1}\right) - n\right]. \tag{I.66}$$

A simpler expression for C is unknown in the general case. Special cases:

(1) $\Sigma_0 = \Sigma_1 = \Sigma$:

$$\mu(s) = -\frac{1}{2}s(1-s)(m_1-m_0)^\top \Sigma^{-1}(m_1-m_0), \tag{I.67}$$

$$B = C = \frac{1}{8}(m_1-m_0)^\top \Sigma^{-1}(m_1-m_0), \tag{I.68}$$

$$D(P_0\|P_1) = D(P_1\|P_0) = \frac{1}{2}(m_1-m_0)^\top \Sigma^{-1}(m_1-m_0). \tag{I.69}$$

C can be solved in this simple case and coincides with B.

(2) If $m_0 = m_1$, the first part in each expression is zero, and B, C, and D can be regarded as distances between two covariance matrices Σ_0 and Σ_1.

(3) Suppose that Σ_0 and Σ_1 commute and $m_0 = m_1$. The two matrices commute if and only if there exists a θ-independent unitary matrix U such that $\Sigma_\theta = UD_\theta U^\dagger$, where $D_{\theta,jk} = \lambda_\theta(j)\delta_{jk}$ is the diagonal matrix of eigenvalues of Σ_θ. Then

$$\mu(s) = -\frac{1}{2}\sum_j \ln \frac{s\lambda_0(j) + (1-s)\lambda_1(j)}{\lambda_0(j)^s \lambda_1(j)^{1-s}}, \tag{I.70}$$

$$B = \frac{1}{2}\sum_j \ln \frac{[\lambda_0(j)+\lambda_1(j)]/2}{\sqrt{\lambda_0(j)\lambda_1(j)}}, \tag{I.71}$$

$$D(P_0\|P_1) = \frac{1}{2}\sum_j \left[\frac{\lambda_1(j)}{\lambda_0(j)} - \ln\frac{\lambda_1(j)}{\lambda_0(j)} - 1\right]. \tag{I.72}$$

These expressions are especially useful if X is a stationary random process, in which case $\lambda_\theta(j)$ is proportional to the power spectral density; see Sec. C.8.

I.7.4. Poisson. Let the observation be the vectoral Poisson random variable $N = (N_1, \dots, N_J) \sim \text{Poisson}(m_\theta)$ with $\mathbb{E}_\theta(N_j) = m_\theta(j)$. Then [63]

$$\mu(s) = \sum_j \left[-sm_1(j) - (1-s)m_0(j) + m_1(j)^s m_0(j)^{1-s}\right], \tag{I.73}$$

$$B = \sum_j \left[\frac{m_0(j)+m_1(j)}{2} - \sqrt{m_1(j)m_0(j)}\right], \tag{I.74}$$

$$D(P_0\|P_1) = \sum_j \left[m_1(j) - m_0(j) + m_0(j)\ln\frac{m_0(j)}{m_1(j)}\right]. \tag{I.75}$$

I.7.5. Joint convexity. Suppose that the probability density of a random variable Y is

$$f_{Y|\theta}(y) = \int f_{Y|X,\theta}(y|x) f_{X|\theta}(x) d\sigma(x), \tag{I.76}$$

where $f_{X|\theta}(x)$ is the probability density of a hidden variable X and $f_{Y|X,\theta}(y|x)$ is the probability density of Y conditioned on $X = x$. We call X the input, Y the output, and the map from $f_{X|\theta}$ to $f_{Y|\theta}$ via $f_{Y|X,\theta}$ a **channel**.

While all the densities may depend on the hypothesis θ in general, we assume in this subsection that the input density $f_{X|0} = f_{X|1} = f_X$ does not. Then the Rényi divergences for a given $s \le 1$ satisfy joint convexity, meaning that $\mu(s)$ for $s \ge 0$ satisfies joint concavity $\mu_Y(s) \ge \mathbb{E}[\mu_{Y|X}(s)]$, while B, C, and D satisfy joint convexity [46]:

$$B_Y \le \mathbb{E}\left(B_{Y|X}\right), \qquad C_Y \le \mathbb{E}\left(C_{Y|X}\right), \qquad D(P_{Y|0}\|P_{Y|1}) \le \mathbb{E}\left[D(P_{Y|X,0}\|P_{Y|X,1})\right], \tag{I.77}$$

where the subscript Y denotes a quantity in terms of the output $f_{Y|\theta}$, the subscript $Y|X$ denotes a quantity in terms of the channel $f_{Y|X,\theta}$, and

$$\mathbb{E}[g(X)] = \int g(x) f_X(x) d\sigma(x) \tag{I.78}$$

is the expectation with respect to the input f_X. Joint convexity means that, if one has access to a hidden random variable X of an experiment, then the distinguishability on average is higher than that without access to X.

I.7.6. Data-processing inequality. Now assume a channel given by Eq. (I.76) that does not depend on θ, i.e., $f_{Y|X,0} = f_{Y|X,1} = f_{Y|X}$. Then the Rényi divergences satisfy the data-processing inequality, implying that our distances also satisfy the inequalities:

$$B_Y \leq B_X, \qquad C_Y \leq C_X, \qquad D(P_{Y|0} \| P_{Y|1}) \leq D(P_{X|0} \| P_{X|1}). \tag{I.79}$$

where the subscript X denotes a quantity in terms of the input $f_{X|\theta}$. The inequality is so called because a channel can model any processing of the input X to produce an output Y. The inequality implies that no postprocessing can increase the distinguishability of two probability measures (as long as the processing has no access to the hypothesis). Another name for a data-processing inequality is monotonicity.

The channel can also model the evolution of an open system in time, where $P_{X|\theta}$ models the initial system state and $P_{Y|\theta}$ models the final state. The data-processing inequality can then be regarded as a generalization of the second law of thermodynamics.

I.7.7. Strong concavity. Define the Bhattacharyya coefficient as

$$\tilde{B} \equiv \exp(-B) = \int \sqrt{f_0(x) f_1(x)} d\sigma(x). \tag{I.80}$$

Then, given Eq. (I.76), where all the densities may depend on θ, $\tilde{B}$ satisfies the strong concavity [47]

$$\tilde{B}_Y \geq \int \tilde{B}_{Y|x} \sqrt{f_{X|0}(x) f_{X|1}(x)} d\sigma(x), \tag{I.81}$$

where $\tilde{B}_{Y|x}$ is the Bhattacharyya coefficient in terms of the channel $f_{Y|X,\theta}$ with $X = x$. In terms of the Bhattacharyya distances,

$$B_Y \leq -\ln \int e^{-B_{Y|x}} \sqrt{f_{X|0}(x) f_{X|1}(x)} d\sigma(x). \tag{I.82}$$

We get back the joint convexity of B if $f_{X|0} = f_{X|1}$ because

$$\int e^{-B_{Y|x}} f_X(x) d\sigma(x) = \mathbb{E}(e^{-B_{Y|X}}) \geq \exp\big[-\mathbb{E}(B_{Y|X})\big], \qquad \text{(Jensen)} \tag{I.83}$$

$$B_Y \leq -\ln \mathbb{E}(e^{-B_{Y|X}}) \leq \mathbb{E}\left(B_{Y|X}\right), \tag{I.84}$$

and we get back the data-processing inequality if $f_{Y|X,0} = f_{Y|X,1}$ so that $B_{Y|X} = 0$.

APPENDIX J

Parameter Estimation*

J.1. Key parameter

Often a model involves a huge number of unknowns but a practitioner is interested only in certain succinct properties of it. For example,

(1) For a vectoral parameter $\theta = (\theta_1, \dots, \theta_p) \in \Theta \subseteq \mathbb{R}^p$, one may be interested in only θ_1 and not the rest $(\theta_2, \dots, \theta_p)$, which are called nuisance parameters.
(2) For a waveform $\theta(t)$ in some function space, one may be interested in only the energy $\int_{-\infty}^{\infty} |\theta(t)|^2 dt$ or the mean arrival time $\int_{-\infty}^{\infty} t|\theta(t)|^2 dt$.
(3) Suppose that we know nothing about the statistical model except the sample/event spaces (Ω, E). Then $P_\theta = \theta \in \Theta$, where Θ is the set of all probability measures. This model is called nonparametric (not the best name as there is still a parameter, namely, the probability measure itself). Given n i.i.d. observations, one may be interested in a population parameter

$$\beta(P) = \int b(x) dP(x). \tag{J.1}$$

Mathematically, we model a large number of unknowns by a high-dimensional parameter space Θ. The statistical model remains $\{P_\theta : \theta \in \Theta\}$, while we define the parameter of interest by a function $\beta : \Theta \to \Phi$. We call $\beta(\theta) \in \Phi$ the **key parameter**, also called the parameter of interest, and Φ the key parameter space. The decision rule, more often called the estimator in parameter estimation, is now taken as $\check{\beta} : \Omega \times \Omega' \to \Phi$, and we should redefine the loss function $l(\beta, \check{\beta})$ in terms of the true $\beta(\theta)$ and the estimate $\check{\beta}(x, y)$. For example, if the key parameter is a real number, we can define the square loss as

$$l(\beta, \check{\beta}) = \left(\beta - \check{\beta}\right)^2. \tag{J.2}$$

It can be proved using the Rao-Blackwell theorem that, for a large class of loss functions including the square loss, ancillas do not help [64], so we assume deterministic estimators $\check{\beta}(x)$ hereafter. The errors are now defined as

$$R(\theta, \check{\beta}) \equiv \int l(\beta(\theta), \check{\beta}(x)) dP_\theta(x), \qquad R_\pi(\check{\beta}) \equiv \int R(\theta, \check{\beta}) d\pi(\theta), \tag{J.3}$$

$$R_{\text{Bayes}} \equiv \min_{\check{\beta}} R_\pi(\check{\beta}), \qquad R_{\text{minimax}} \equiv \min_{\check{\beta}} \max_{\theta} R(\theta, \check{\beta}), \tag{J.4}$$

and we can rewrite Eq. (H.26) as

$$R_{\text{minimax}} = \max_{\theta \in \Theta} R(\theta, \check{\beta}_{\text{minimax}}) \geq R_\pi(\check{\beta}_{\text{minimax}}) \geq \min_{\check{\beta}} R_\pi(\check{\beta}) = R_{\text{Bayes}}(\pi). \tag{J.5}$$

We get back the simpler-looking formalism in Chap. H if we set $\beta(\theta) = \theta$. Conversely, we can also obtain the key-parameter formalism here as a special case of the one in Chap. H if we define a larger parameter space as the graph of β

$$\{(\theta, \phi) \in \Theta \times \Phi : \phi = \beta(\theta)\} \tag{J.6}$$

and require the loss function to depend only on the ϕ component of the augmented parameter (θ, ϕ).

A practical reason for introducing the key-parameter concept is that an accurate estimation of a high-dimensional θ is often impossible or infeasible, while the estimation of a low-dimensional $\beta(\theta)$ may be more straightforward.

For example, for the population parameter given by Eq. (J.1), a common estimator is the sample mean

$$\check{\beta}(x_1, \dots, x_n) = \frac{1}{n}\sum_{j=1}^{n} b(x_j), \tag{J.7}$$

and there is no need to estimate the underlying measure P.

J.2. Bayes estimator

The Bayesian theory is the cleanest so we start with it. For simplicity, assume that β is a real number ($\Phi \subseteq \mathbb{R}$); generalizations for a vectoral β are straightforward but too tedious to write out. The error for the square loss is called the **mean square error (MSE)**, defined as

$$R(\theta, \check{\beta}) = \int \left[\check{\beta}(x) - \beta(\theta)\right]^2 dP_\theta(x) = \mathbb{E}_\theta\left\{\left[\check{\beta} - \beta(\theta)\right]^2\right\}, \tag{J.8}$$

while we call

$$R_\pi(\check{\beta}) = \int R(\theta, \check{\beta}) d\pi(\theta) = \mathbb{E}\left[\left(\check{\beta} - \beta\right)^2\right] \tag{J.9}$$

the average MSE, which is obtained after taking the expectation $\mathbb{E}$ with respect to both the observation x and the parameter θ. The scalar β, the square loss, and the MSE's are assumed hereafter in this chapter.

The Bayes estimator here is also called the minimum-MSE (MMSE) estimator, and it is given by the conditional expectation

$$\check{\beta}_{\text{Bayes}}(x) = \int \beta(\theta) dQ_x(\theta), \tag{J.10}$$

where Q_x is the posterior measure described in Sec. H.7. The resulting Bayes error has the interesting formula

$$R_{\text{Bayes}}(\pi) \equiv \min_{\check{\beta}} R_\pi(\check{\beta}) = R_\pi(\check{\beta}_{\text{Bayes}}) = \mathbb{V}(\beta) - \mathbb{V}(\check{\beta}_{\text{Bayes}}) = \mathbb{E}\left(\beta^2\right) - \mathbb{E}\left(\check{\beta}^2_{\text{Bayes}}\right), \tag{J.11}$$

$$\mathbb{E}\left(\beta^2\right) = \int \beta(\theta)^2 d\pi(\theta), \quad \mathbb{E}\left(\check{\beta}^2_{\text{Bayes}}\right) = \int \check{\beta}_{\text{Bayes}}(x)^2 dP_\theta(x) d\pi(\theta), \tag{J.12}$$

$$\mathbb{E}(\beta) = \int \beta(\theta) d\pi(\theta) = \mathbb{E}(\check{\beta}_{\text{Bayes}}) = \int \check{\beta}_{\text{Bayes}}(x) dP_\theta(x) d\pi(\theta), \tag{J.13}$$

where $\mathbb{V}$ denotes the variance with respect to $dP_\theta(x)d\pi(\theta)$ and Eq. (J.13) follows from the law of total expectation (see Appendix C).

Side note. *Eq. (J.11) looks like a Pythagorean theorem, and indeed the average MSE and the conditional expectation that minimizes it have a geometric interpretation [65].*

Eq. (J.11) in itself is not very useful, but we can at least read from it a trivial upper bound

$$R_{\text{Bayes}} \leq \mathbb{V}(\beta) \tag{J.14}$$

given by the prior variance $\mathbb{V}(\beta)$. The right-hand side is equal to the average error $R_\pi(\check{\beta})$ if we set the estimator $\check{\beta}(x)$ to be the prior expected value $\mathbb{E}(\beta)$, ignoring any observation x. An experiment is informative only when the average error is much lower than than the prior variance, so we need alternative ways to evaluate R_{Bayes}.

J.3. Linear Gaussian model

A rare case where $\check{\beta}_{\text{Bayes}}(x)$ and the Bayes MSE R_{Bayes} can be evaluated exactly is when the observation and the prior follow the linear Gaussian model and the key parameter is a linear function of $\theta \in \Theta = \mathbb{R}^p$:

$$x \sim \mathcal{N}(A\theta, \Sigma) \text{ under } P_\theta, \qquad \theta \sim \mathcal{N}(\bar{\theta}, \Pi) \text{ under } \pi, \qquad \beta(\theta) = b^\top \theta, \tag{J.15}$$

where A is an $m \times p$ matrix, Σ is the $m \times m$ observation covariance matrix, $\bar{\theta}$ is the prior mean ($p \times 1$ column vector), Π is the prior covariance matrix, and b is a $p \times 1$ column vector, all assumed to be independent of θ (we've

abused notation by using x and θ to denote the random variables as well). Then the posterior measure Q_x is also Gaussian:

$$\theta \sim \mathcal{N}(\check{\theta}_{\text{Bayes}}(x), \Upsilon) \text{ under } Q_x, \quad \check{\theta}_{\text{Bayes}}(x) = \Upsilon\left(A^\top \Sigma^{-1} x + \Pi^{-1}\bar{\theta}\right), \quad \Upsilon \equiv \left(A^\top \Sigma^{-1} A + \Pi^{-1}\right)^{-1}. \tag{J.16}$$

The posterior mean $\check{\theta}_{\text{Bayes}}$ is a weighted average of the observation x and the prior $\bar{\theta}$, while the inverse posterior covariance Υ^{-1} is a weighted sum of the inverse observation covariance Σ^{-1} and the inverse prior covariance Π^{-1}. For the estimation of $\beta = b^\top \theta$, we obtain

$$\check{\beta}_{\text{Bayes}}(x) = b^\top \check{\theta}_{\text{Bayes}}(x), \tag{J.17}$$

$$\boxed{R_{\text{Bayes}} = b^\top \Upsilon b.} \tag{J.18}$$

The famous Wiener and Kalman filters assume this linear Gaussian model. The Kalman filter and its extensions have found many successful applications in diverse areas of science and engineering, most notably in navigation (https://en.wikipedia.org/wiki/Kalman_filter).

J.4. Bayes error bounds

J.4.1. Gill-Levit bounds. R_{Bayes} is difficult to compute in most cases, and we often have to resort to error bounds. There are a whole zoo of lower error bounds in the literature [66]; here we mention just one family of bounds called the Gill-Levit bounds [67], also called Bayesian Cramér-Rao bounds or Van Trees inequalities, which include many useful bounds as special cases.

Side note. *Beware that the Gill-Levit bounds may grossly underestimate R_{Bayes} for certain problems. See, for example, Ref. [66] for alternative bounds that may work better.*

Let $\varrho(\theta)$ be the probability density of the prior π (with respect to the Lebesgue measure). Assume that ϱ is strictly positive, i.e., $\varrho(\theta) > 0$ for all $\theta \in \Theta$. Let

$$\nabla \equiv \begin{pmatrix} \frac{\partial}{\partial \theta_1} & \cdots & \frac{\partial}{\partial \theta_p} \end{pmatrix}^\top \tag{J.19}$$

be the gradient with respect to θ. Assume also that each observation density $f_\theta(x)$ is strictly positive for all $x \in \Omega$. Then the Gill-Levit bounds on the average MSE for a scalar $\beta : \Theta \to \mathbb{R}$ are given by

$$\boxed{R_\pi(\check{\beta}) \geq G(v) \equiv \frac{[\mathbb{E}(v \cdot \nabla \beta)]^2}{\mathbb{E}\left[v^\top F v + (\operatorname{div}_\varrho v)^2\right]},} \tag{J.20}$$

$$\mathbb{E}(\dots) = \int (\dots) d\pi(\theta) = \int (\dots) \varrho(\theta) d^p\theta, \tag{J.21}$$

$$v(\theta) \cdot \nabla \beta(\theta) = \sum_j v_j(\theta) \frac{\partial \beta(\theta)}{\partial \theta_j}, \tag{J.22}$$

$$v(\theta)^\top F(\theta) v(\theta) = \sum_{j,k} v_j(\theta) F_{jk}(\theta) v_k(\theta), \tag{J.23}$$

$$\boxed{F_{jk}(\theta) \equiv \mathbb{E}_\theta\left[\left(\frac{\partial}{\partial \theta_j} \ln f_\theta\right)\left(\frac{\partial}{\partial \theta_k} \ln f_\theta\right)\right] = \int \left[\frac{\partial}{\partial \theta_j} \ln f_\theta(x)\right]\left[\frac{\partial}{\partial \theta_k} \ln f_\theta(x)\right] f_\theta(x) d\sigma(x),} \tag{J.24}$$

$$\operatorname{div}_\varrho v(\theta) \equiv \frac{1}{\varrho(\theta)} \nabla \cdot [\varrho(\theta) v(\theta)] = \frac{1}{\varrho(\theta)} \sum_j \frac{\partial}{\partial \theta_j} [\varrho(\theta) v_j(\theta)]. \tag{J.25}$$

The proof is in Sec. J.8 and the quantities are defined as follows:

(1) $v : \Theta \to \mathbb{R}^p$ is any vector field on the parameter space Θ that satisfies

$$\varrho(\theta) v(\theta) = 0 \quad \forall \theta \in \text{boundary}(\Theta). \tag{J.26}$$

(2) F given by Eq. (J.24) is called the **Fisher information matrix**. It is the only term in the bound that depends on the observation densities $\{f_\theta(x)\}$. Another handy formula is

$$F_{jk}(\theta) = \mathbb{E}_\theta\left(-\frac{\partial^2}{\partial\theta_j\partial\theta_k}\ln f_\theta\right) = \int\left[-\frac{\partial^2}{\partial\theta_j\partial\theta_k}\ln f_\theta(x)\right]f_\theta(x)d\sigma(x). \tag{J.27}$$

The Fisher information is a fundamental metric of the statistical model; more on that later.

(3) $\operatorname{div}_\varrho v$ depends on the vector field $v(\theta)$ and the prior density $\varrho(\theta)$ only.

Note that

(1) The bound $G(v)$ does not depend on the estimator and applies also to the Bayes error $R_{\text{Bayes}} = R_\pi(\check\beta_{\text{Bayes}})$.
(2) By virtue of Eq. (J.5), $G(v)$ for any prior π also serves as a lower bound on the minimax error R_{minimax} as well as the worst-case error $\max_\theta R(\theta,\check\beta)$ for any estimator.
(3) By choosing the vector field v, we can obtain various bounds useful for different purposes.
(4) Given a v, cv for any nonzero constant c gives the same bound.

Side note. *It is possible to reframe $G(v)$ in the language of differential geometry and treat $\varrho(\theta)$, $v(\theta)$, $F(\theta)$, and ∇ as geometric concepts on a manifold Θ [68, 69].*

J.4.2. Optimal Gill-Levit bound. An optimal choice of v to give the highest Gill-Levit bound $\max_v G(v)$ can be obtained by solving the linear partial differential equation [69]

$$Tv(\theta) \equiv F(\theta)v(\theta) - \nabla[\operatorname{div}_\varrho v(\theta)] = \nabla\beta(\theta), \tag{J.28}$$

where T is a linear operator, assuming that a solution exists ($\nabla\beta$ is in the range of T). Any solution gives the same bound, and writing it as $v = T^{-1}\nabla\beta$, the optimal bound is

$$\max_v G(v) = \mathbb{E}\left[(\nabla\beta)^\top\left(T^{-1}\nabla\beta\right)\right], \tag{J.29}$$

as proved in Sec. J.8.

J.4.3. Schützenberger-Van Trees bound. Let v be the constant vector field

$$v = [\mathbb{E}(F+H)]^{-1}\,\mathbb{E}(\nabla\beta), \qquad H_{jk}(\theta) \equiv -\frac{\partial^2}{\partial\theta_j\partial\theta_k}\ln\varrho(\theta). \tag{J.30}$$

Then the bound becomes

$$\boxed{G(v) = \mathbb{E}(\nabla\beta)^\top[\mathbb{E}(F+H)]^{-1}\,\mathbb{E}(\nabla\beta).} \tag{J.31}$$

This bound was first discovered by Schützenberger in 1957 [70] and then independently by Van Trees [55, 66]. The $H(\theta)$ matrix depends on the prior density $\varrho(\theta)$ only and quantifies the prior information, similar to the Fisher information matrix $F(\theta)$.

The bound coincides with the optimal Gill-Levit bound if $\nabla\beta(\theta)$ and $F(\theta)$ are constant and $\varrho(\theta)$ is Gaussian, such that $H = \Pi^{-1}$ is the inverse of the prior covariance matrix and the v given by Eq. (J.30) satisfies Eq. (J.28).

For the linear Gaussian model in Sec. J.3, the Schützenberger-Van Trees bound coincides with the Bayes error given by Eq. (J.18), since

$$\mathbb{E}(\nabla\beta) = \nabla\beta = b, \quad \mathbb{E}(F) = F = A^\top\Sigma^{-1}A, \quad \mathbb{E}(H) = H = \Pi^{-1}, \quad \mathbb{E}(F+H) = F + H = \Upsilon^{-1}. \tag{J.32}$$

Of course, we don't need any error bound for the linear Gaussian model since we know the error exactly. What this example offers is an intuition: the bound should be pretty good if the model is close to linear Gaussian.

J.4.4. Borovkov-Sakhanenko bound. For n i.i.d. observations, the total Fisher information

$$\boxed{F^{(n)}(\theta) = nF(\theta)} \tag{J.33}$$

is n times $F(\theta)$ of one observation, and we pick

$$v(\theta) = F(\theta)^{-1}\nabla\beta(\theta), \tag{J.34}$$

so that

$$v(\theta)\cdot\nabla\beta(\theta) = v(\theta)^\top F(\theta)v(\theta) = \boxed{[\nabla\beta(\theta)]^\top F(\theta)^{-1}\nabla\beta(\theta) \equiv \mathsf{C}(\theta).} \tag{J.35}$$

$\operatorname{div}_\varrho v$ does not depend on n and does not need to be written out explicitly here. The resulting bound $G^{(n)}(v)$ is called the Borovkov-Sakhanenko bound [71], given by

$$G^{(n)}(v) = \frac{[\mathbb{E}(\mathsf{C})]^2}{n\,\mathbb{E}(\mathsf{C}) + \mathbb{E}[(\operatorname{div}_\varrho v)^2]} \geq \frac{1}{n}\,\mathbb{E}(\mathsf{C}) - \frac{1}{n^2}\,\mathbb{E}[(\operatorname{div}_\varrho v)^2] \qquad (1/(1+u) \geq 1-u) \tag{J.36}$$

$$= \boxed{\frac{\mathbb{E}(\mathsf{C})}{n} + o\left(\frac{1}{n}\right).} \tag{J.37}$$

This bound is important because $\mathsf{C}(\theta)/n$ turns out to coincide with the Cramér-Rao bound (CRB) and also the asymptotic error of the maximum-likelihood (ML) estimator, both historically important concepts to be tackled in Secs. J.5 and J.6.

J.4.5. Upper bounds. Curiously, upper error bounds for parameter estimation are not as well studied, although I can present one family here. Let $\Omega \subseteq \mathbb{R}^n$ and assume that the estimator

$$\check\beta_D(x) = \sum_{d=0}^{D}\sum_{j_1,\ldots,j_l} c^{(d)}_{j_1,\ldots,j_l} x_{j_1}\ldots x_{j_d} \tag{J.38}$$

$$= c^{(0)} + \sum_{j_1} c^{(1)}_{j_1}x_{j_1} + \sum_{j_1,j_2} c^{(2)}_{j_1j_2}x_{j_1}x_{j_2} + \cdots + \sum_{j_1,\ldots,j_D} c^{(D)}_{j_1,\ldots,j_D}x_{j_1}\ldots x_{j_D} \tag{J.39}$$

is a degree-D polynomial of the observation x called the Volterra filter or the polynomial filter [72]. If we define

$$y = \begin{pmatrix}1, & x_1, & \ldots & x_n, & \ldots & x_{j_1}\ldots x_{j_d}, & \ldots\end{pmatrix}^\top \tag{J.40}$$

as a column vector of all the monomials of x up to degree D, then the estimator can be expressed as

$$\check\beta_D = c^\top y, \tag{J.41}$$

where c is a column vector. The average error becomes

$$R_\pi(\check\beta_D) = \mathbb{E}\left[\left(c^\top y - \beta\right)^2\right] = c^\top\,\mathbb{E}\left(yy^\top\right)c - 2c^\top\,\mathbb{E}(y\beta) + \mathbb{E}(\beta^2). \tag{J.42}$$

The optimal c is then

$$c = \left[\mathbb{E}\left(yy^\top\right)\right]^{-1}\mathbb{E}(y\beta), \qquad R_\pi(\check\beta_D) = \mathbb{E}(\beta^2) - \mathbb{E}(y\beta)^\top\left[\mathbb{E}\left(yy^\top\right)\right]^{-1}\mathbb{E}(y\beta) \geq R_{\text{Bayes}}. \tag{J.43}$$

The simplest example is when $D = 0$, $\check\beta_0 = \mathbb{E}(\beta)$, and we obtain the trivial $R_\pi = \mathbb{V}(\beta)$. It is equal to R_{Bayes} when the observation is independent of the parameter and the optimal estimator is simply the prior expectation. The next simplest example is when $D = 1$ and the estimator is linear. For the linear Gaussian model in Sec. J.3, we know that a linear estimator is optimal among all estimators, so $R_\pi(\check\beta_1) = R_{\text{Bayes}}$, and the upper bound is tight. For other models, $R_\pi(\check\beta_1)$ may be the easiest nontrivial upper bound.

In general, $R_\pi(\check\beta_D)$ decreases with D ($R_\pi(\check\beta_D) \geq R_\pi(\check\beta_{D'})$ for $D < D'$), so one may try to improve the upper bound by increasing D. One may also put different functions of x in y other than monomials.

J.5. Maximum-likelihood (ML) estimator

We now switch gears to the frequentist approach, ignoring any prior. We could go the minimax route, but it is too difficult a subject to be addressed in this book; see Refs. [53, 73] for example. Instead, here we will focus on the most popular estimator in frequentist statistics called the maximum-likelihood (ML) estimator.

To define the estimator, let us plug the observation x into the observation probability densities $f_\theta(x)$. $f_\theta(x)$ as a function of the parameter θ is called the **likelihood function**. (We've encountered this function earlier in Chap. I in the context of the likelihood ratio $f_1(x)/f_0(x)$.) In terms of the likelihood function, the maximum-likelihood (ML) estimator is defined as

$$\boxed{\check{\beta}_{\text{ML}}(x) \equiv \beta(\check{\theta}_{\text{ML}}(x)),} \qquad\qquad \boxed{\check{\theta}_{\text{ML}}(x) \equiv \arg\max_\phi f_\phi(x),} \tag{J.44}$$

where we've used a different variable ϕ for the argument of the likelihoood function, reserving θ for the true parameter.

Elementary properties of the maximization:

(1)
$$\arg\max_\phi f_\phi(x) = \arg\max_\phi \ln f_\phi(x) \tag{J.45}$$
in terms of the log-likelihood $\ln f_\phi(x)$; the latter is often easier to solve.

(2) We are free to add any ϕ-independent term $g(x)$ to the function $f_\phi(x)$ or $\ln f_\phi(x)$ to be maximized; it doesn't change the maximum point $\arg\max$.

(3) We can also multiply the function $f_\phi(x)$ or $\ln f_\phi(x)$ by any positive ϕ-independent term.

(4) If we multiply $f_\phi(x)$ or $\ln f_\phi(x)$ by -1, we can use $\arg\min_\phi$ instead of $\arg\max_\phi$.

The ML estimator is hard to study in general but its asymptotic properties are easier to derive; we present a quick and dirty derivation in the following.

J.5.1. Consistency. For n i.i.d. observations $(x_1, \ldots, x_n)$, write

$$\check{\theta}^{(n)}_{\text{ML}}(x_1, \ldots, x_n) = \arg\max_\phi L^{(n)}_\phi(x_1, \ldots, x_n), \tag{J.46}$$

where

$$L^{(n)}_\phi(x_1, \ldots, x_n) \equiv \frac{1}{n}\sum_{j=1}^n \ln f_\phi(x_j) \tag{J.47}$$

is the sample mean of the log-likelihood random variable

$$L_\phi(x) \equiv L^{(1)}_\phi(x) = \ln f_\phi(x). \tag{J.48}$$

Let θ be the true parameter. For $n \to \infty$, the law of large numbers gives

$$L^{(n)}_\phi \to \mathbb{E}_\theta\left(L_\phi\right) = \mathbb{E}_\theta\left(L_\theta\right) - D(P_\theta \| P_\phi), \qquad D(P_\theta\|P_\phi) = \int \ln\frac{f_\theta(x)}{f_\phi(x)} f_\theta(x) d\sigma(x). \tag{J.49}$$

Since the relative entropy obeys $D \geq 0$ and gives $D = 0$ if and only if $P_\theta = P_\phi$,

$$\arg\max_\phi \mathbb{E}_\theta\left(L_\phi\right) = \theta \tag{J.50}$$

as long as $\theta \neq \phi$ implies $P_\theta \neq P_\phi$ (in which case we say θ is identifiable). Hence, we expect the estimator to converge to the true parameter:

$$\check{\theta}^{(n)}_{\text{ML}} \equiv \arg\max_\phi L^{(n)}_\phi \to \arg\max_\phi \mathbb{E}_\theta\left(L_\phi\right) = \theta, \tag{J.51}$$

$$\check{\beta}^{(n)}_{\text{ML}} \equiv \beta\left(\check{\theta}^{(n)}_{\text{ML}}\right) \to \beta(\theta). \tag{J.52}$$

An estimator is said to be consistent if $\check{\beta}^{(n)} \to \beta$, so the ML estimator is consistent.

J.5.2. Asymptotic bias. Consistency implies that the peak location $\check{\theta}^{(n)}_{\text{ML}} \equiv \arg\max_\phi L^{(n)}_\phi$ of $L^{(n)}_\phi$ will be pretty close to the true θ for a large enough n. To study the behavior of $\check{\theta}^{(n)}_{\text{ML}}$ in that case, we approximate $L^{(n)}_\phi$ for a ϕ close to θ by the Taylor series

$$L^{(n)}_\phi \approx L^{(n)}_\theta + (\phi-\theta)^\top \nabla L^{(n)}_\theta + \frac{1}{2}(\phi-\theta)^\top \left(\nabla\nabla^\top L^{(n)}_\theta\right)(\phi-\theta) \tag{J.53}$$

$$\approx L^{(n)}_\theta + (\phi-\theta)^\top \nabla L^{(n)}_\theta - \frac{1}{2}(\phi-\theta)^\top F(\theta)(\phi-\theta), \tag{J.54}$$

where we have made the approximation

$$\nabla\nabla^\top L^{(n)}_\theta = \frac{1}{n}\sum_{j=1}^n \nabla\nabla^\top \ln f_\theta(x_j) \approx \mathbb{E}_\theta\left(\nabla\nabla^\top \ln f_\theta\right) \qquad \text{(law of large numbers)} \tag{J.55}$$

$$= -F(\theta) \tag{J.56}$$

and F is the Fisher information in Eq. (J.27) for one observation. The Taylor series means that $L^{(n)}_\phi$ is approximately quadratic with respect to ϕ. Maximizing the quadratic function gives

$$\check{\theta}^{(n)}_{\text{ML}} \equiv \arg\max_\phi L^{(n)}_\phi \approx \theta + F(\theta)^{-1}\nabla L^{(n)}_\theta, \tag{J.57}$$

$$\check{\beta}^{(n)}_{\text{ML}} \approx \beta(\theta) + [\nabla\beta(\theta)]^\top\left(\check{\theta}^{(n)}_{\text{ML}} - \theta\right) \approx \beta(\theta) + [\nabla\beta(\theta)]^\top F(\theta)^{-1}\nabla L^{(n)}_\theta. \tag{J.58}$$

Define the bias of an estimator as

$$\delta(\theta) \equiv \mathbb{E}_\theta\left(\check{\beta}\right) - \beta(\theta). \tag{J.59}$$

Then the bias of the ML estimator is

$$\delta^{(n)}_{\text{ML}}(\theta) \equiv \mathbb{E}_\theta\left(\check{\beta}^{(n)}_{\text{ML}}\right) - \beta \approx [\nabla\beta(\theta)]^\top F(\theta)^{-1}\,\mathbb{E}_\theta\left(\nabla L^{(n)}_\theta\right) = 0, \tag{J.60}$$

since

$$\mathbb{E}_\theta\left(\nabla L^{(n)}_\theta\right) = \mathbb{E}_\theta\left(\nabla L_\theta\right) = \int [\nabla \ln f_\theta(x)] f_\theta(x) d\sigma(x) = \int [\nabla f_\theta(x)] d\sigma(x) \tag{J.61}$$

$$= \nabla \int f_\theta(x) d\sigma(x) = \nabla(1) = 0, \tag{J.62}$$

where we have pulled the gradient ∇ with respect to θ out of the integral with respect to x. It can in fact be proved more rigorously that the ML estimator is asymptotically unbiased [74], viz.,

$$\delta^{(n)}_{\text{ML}}(\theta) \to 0. \tag{J.63}$$

J.5.3. Asymptotic error. Eq. (J.58) also gives

$$R\left(\theta, \check{\beta}^{(n)}_{\text{ML}}\right) \equiv \mathbb{E}_\theta\left\{\left[\check{\beta}^{(n)}_{\text{ML}} - \beta(\theta)\right]^2\right\} \tag{J.64}$$

$$\approx [\nabla\beta(\theta)]^\top F(\theta)^{-1}\,\mathbb{E}_\theta\left[\left(\nabla L^{(n)}_\theta\right)\left(\nabla L^{(n)}_\theta\right)^\top\right] F(\theta)^{-1}\nabla\beta(\theta) \tag{J.65}$$

$$= \frac{1}{n}[\nabla\beta(\theta)]^\top F(\theta)^{-1}\nabla\beta(\theta) \equiv \frac{\mathsf{C}(\theta)}{n}. \tag{J.66}$$

All the rough arguments thus far can be proved a lot more rigorously under a subject called local asymptotic normality [74], which states that the random variable $\sqrt{n}(\check{\theta}^{(n)}_{\text{ML}} - \theta)$ converges to a normal random variable $\mathcal{N}(0, F(\theta)^{-1})$. A more precise statement of Eq. (J.66) becomes

$$r(\theta, \check{\beta}_{\text{ML}}) \equiv \lim_{n\to\infty} nR\left(\theta, \check{\beta}^{(n)}_{\text{ML}}\right) = \mathsf{C}(\theta), \tag{J.67}$$

or, equivalently,

$$\boxed{R\Big(\theta, \check{\beta}^{(n)}_{\text{ML}}\Big) = \frac{\mathsf{C}(\theta)}{n} + o\Big(\frac{1}{n}\Big).} \tag{J.68}$$

The resulting average error

$$R_\pi\Big(\check{\beta}^{(n)}_{\text{ML}}\Big) = \frac{\mathbb{E}\,(\mathsf{C})}{n} + o\Big(\frac{1}{n}\Big) \tag{J.69}$$

approaches the Borovkov-Sakhanenko bound given by Eq. (J.37) if we ignore all the $o(1/n)$ terms. Hence, under the conditions for the bound and the error (such as the strict positivity of the densities ϱ and f_θ, the existence of F^{-1}, and the identifiability of θ), the ML estimator is asymptotically optimal in the sense of

$$\lim_{n\to\infty} nR_\pi\Big(\check{\beta}^{(n)}_{\text{ML}}\Big) = \lim_{n\to\infty} nG^{(n)}(v). \tag{J.70}$$

Note that there is no limit on the absolute size of the $o(1/n)$ term in Eq. (J.68), only that it decays faster than $1/n$, i.e., $no(1/n) \to 0$. For any finite n, Eq. (J.68) is not at all precise about the absolute error of the ML estimator. Moreover, the $o(1/n)$ term may depend on θ, and the convergence $no(1/n) \to 0$ is pointwise, not uniform, meaning that the $o(1/n)$ term for a given finite n may be negligible for some θ but not for others. Note also that $o(1/n)$ may be positive or negative. Just like Stein's lemma in Sec. I.5, asymptotic statements should be treated with caution.

It is also possible that $\mathsf{C}(\theta) = \infty$, in which case the asymptotic theory here breaks down. It means that $nR \to \infty$, and R is decaying more slowly than the $1/n$ trend.

J.6. Cramér-Rao bound (CRB)

The Cramér-Rao bound (CRB) is one of the earliest error bounds in statistics and still remains very popular today. However, it makes questionable assumptions about the estimator bias and is not as conclusive as the Bayesian error bounds, so we present it last.

Let us focus on the error at the true θ and decompose the MSE as

$$R(\theta, \check{\beta}) = \mathbb{V}_\theta(\check{\beta}) + \delta(\theta)^2, \qquad \mathbb{V}_\theta(\check{\beta}) \equiv \mathbb{E}_\theta\Big\{\big[\check{\beta} - \bar{\beta}(\theta)\big]^2\Big\}, \qquad \delta(\theta) \equiv \bar{\beta}(\theta) - \beta(\theta), \tag{J.71}$$

where we have defined

$$\bar{\beta}(\theta) \equiv \mathbb{E}_\theta(\check{\beta}) \tag{J.72}$$

as the mean of the estimator. Then Sec. J.8 proves that

$$R(\theta, \check{\beta}) \geq \mathbb{V}_\theta(\check{\beta}) \geq \big[\nabla\bar{\beta}(\theta)\big]^\top F(\theta)^{-1}\nabla\bar{\beta}(\theta). \tag{J.73}$$

This bound in itself is rather useless, since $\bar{\beta}(\theta)$ depends on the estimator $\check{\beta}$ and there is no lower limit on the magnitude of $\nabla\bar{\beta}$; we might as well compute the error $R(\theta, \check{\beta})$ directly if we have to specify an estimator. However, if we assume that the estimator is unbiased around the true θ, i.e.,

$$\bar{\beta}(\theta) = \beta(\theta), \qquad \nabla\bar{\beta}(\theta) = \nabla\beta(\theta), \tag{J.74}$$

then we obtain the CRB

$$\boxed{R(\theta, \check{\beta}) = \mathbb{V}_\theta(\check{\beta}) \geq [\nabla\beta(\theta)]^\top F(\theta)^{-1}\nabla\beta(\theta) \equiv \mathsf{C}(\theta).} \tag{J.75}$$

C already appeared in two places earlier: the Borovkov-Sakhanenko bound in Eq. (J.37) and the asymptotic error of the ML estimator in Eq. (J.68). We find here a third significance for $\mathsf{C}(\theta)$: it is also a lower error bound for any unbiased estimator. An unbiased estimator is called efficient if its error achieves the CRB.

Exercise J.1. Derive the bounds in this section of wikipedia: https://en.wikipedia.org/wiki/Cram%C3%A9r%E2%80%93Rao_bound#Bound_on_the_variance_of_biased_estimators.

Remark J.1. *Eqs. (J.74) at one point θ are called the local unbiased condition, which is sufficient to yield the CRB at that point. Technically speaking, the condition allows the estimator to be biased at other points of the parameter space. But of course θ is unknown in practice; allowing an estimator to be biased outside an unknown point is not much of a generalization.*

Despite the name "bias" suggesting that it is a bad thing we should minimize, if we think about it, there is no good reason why we should care about the estimator mean $\bar{\beta}$ and why the bias should be zero so that the estimator mean $\bar{\beta}$ is equal to the true parameter β. All one should care about is how close the estimator $\check{\beta}$ is to β, as quantified by the error $R(\theta, \check{\beta})$. It makes no difference in practice whether the error is dominated by the variance $\mathbb{V}_\theta(\check{\beta})$ or the squared bias $\delta(\theta)^2$, and a biased estimator may have a lower error afterall. Moreover, exactly unbiased estimators may not even exist for a problem and many standard estimators may be biased; even the ML estimator may be biased. For a finite n, it is entirely possible for a biased estimator, such as the ML estimator, to have an error $R(\theta, \check{\beta})$ that violates the CRB $\mathsf{C}(\theta)$ by any amount in certain regions of the parameter space; see Ref. [75] for an example.

To relax the unbiased assumption slightly, consider n i.i.d. observations and allow an estimator $\check{\beta}^{(n)}$ to be only **asymptotically unbiased**:

$$\delta^{(n)}(\theta) \equiv \mathbb{E}_\theta(\check{\beta}^{(n)}) - \beta(\theta) \to 0, \qquad \bar{\beta}^{(n)}(\theta) \equiv \mathbb{E}_\theta(\check{\beta}^{(n)}) \to \beta(\theta). \tag{J.76}$$

The ML estimator now satisfies this relaxed condition. Eq. (J.73) then gives an asymptotic version of the CRB:

$$\boxed{r(\theta, \check{\beta}) \equiv \lim_{n\to\infty} nR(\theta, \check{\beta}^{(n)}) \geq \mathsf{C}(\theta).} \tag{J.77}$$

An estimator $\check{\beta}$ with an asymptotic scaled error $r(\theta, \check{\beta})$ that achieves the CRB $\mathsf{C}(\theta)$ for all θ is called asymptotically efficient. The ML estimator is asymptotically efficient by virtue of Eq. (J.67).

The CRB given by Eq. (J.77) is, again, an asymptotic statement that should be treated with caution. The definition of r means that

$$R(\theta, \check{\beta}^{(n)}) = \frac{r(\theta, \check{\beta})}{n} + o\left(\frac{1}{n}\right). \tag{J.78}$$

For any finite n, there is no limit on the absolute size of the $o(1/n)$ term, and an asymptotically unbiased estimator may still be biased so that it may violate the CRB $\mathsf{C}(\theta)/n$ by any amount. Moreover, the asymptotic unbiased condition is difficult to check, and one may be better off with the Bayesian bounds in Sec. J.4, which do not assume anything about the estimator.

Despite all the caveats, the CRB remains the most popular error bound in statistics and widely accepted as a performance metric of experiments in optics, especially in fluorescence microscopy. For a lot of problems, the CRB often remains tractable while other error bounds are much harder to compute. As long as one is aware of its precise significance and shortcomings, the CRB serves as a decent first option.

J.7. Properties of Fisher information

In view of the fundamental role of the Fisher information in the error bounds and the asymptotics of the ML estimator, it is often used as a performance metric of experiments for parameter estimation. We list some of its properties in the following that can help us compute or bound it.

J.7.1. Relations with Bhattacharyya distance B and relative entropy D. Let $\theta, \phi \in \Theta \subseteq \mathbb{R}^p$ and the Bhattacharyya distance between two measures P_θ and P_ϕ be $B(P_\theta \| P_\phi)$, as introduced in Sec. I.6. If the two parameters θ, ϕ are neighbors, it turns out that B can be approximated as

$$B(P_\theta \| P_{\theta+\epsilon v}) = \frac{1}{8}\epsilon^2 v^\top F(\theta) v + o(\epsilon^2), \qquad F_{jk}(\theta) = 4\,\frac{\partial^2}{\partial\phi_j \partial\phi_k} B(P_\theta \| P_\phi)\bigg|_{\phi=\theta}. \tag{J.79}$$

Similarly, the relative entropy introduced in Chap. I can be approximated as

$$D(P_\theta \| P_{\theta+\epsilon v}) = \frac{1}{2}\epsilon^2 v^\top F(\theta) v + o(\epsilon^2), \qquad F_{jk}(\theta) = \frac{\partial^2}{\partial\phi_j \partial\phi_k} D(P_\theta \| P_\phi)\bigg|_{\phi=\theta}. \tag{J.80}$$

Hence, we can think of F as a metric that determines the distance between two neighboring probability measures.

Side note. *The Fisher information matrix can in fact be regarded as a Riemannian metric for a manifold of probability distributions, as first proposed by Rao [76]. The treatment of statistical distance measures in the language of differential geometry is known as information geometry [77].*

J.7.2. n independent observations. Let $(x_1, \dots, x_n) \in \Omega^n$ be n independent observations following the product probability measure given by Eq. (I.60) and $F_j(\theta)$ be the Fisher information in the jth observation with respect to $\{P_{\theta,j} : \theta \in \Theta\}$. Then the total Fisher information is simply the sum

$$F^{(n)}(\theta) = \sum_j F_j(\theta). \tag{J.81}$$

If the individual measures are identical with $P_{\theta,j} = P_\theta$ and $F_j(\theta) = F(\theta)$, then we get back Eq. (J.33).

J.7.3. Gaussian. Let the observation be the vectoral normal $X \sim \mathcal{N}(m_\theta, \Sigma_\theta)$. Then [78]

$$F_{jk}(\theta) = \left(\frac{\partial m_\theta}{\partial \theta_j}\right)^\top \Sigma_\theta^{-1} \frac{\partial m_\theta}{\partial \theta_k} + \frac{1}{2} \operatorname{tr}\left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_j} \Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_k}\right). \tag{J.82}$$

J.7.4. Poisson. Let the observation be the Poisson $N \equiv (N_1, \dots, N_J) \sim \text{Poisson}(m_\theta)$. Then

$$F_{jk}(\theta) = \sum_l m_\theta(l) \left[\frac{\partial}{\partial \theta_j} \ln m_\theta(l)\right] \left[\frac{\partial}{\partial \theta_k} \ln m_\theta(l)\right]. \tag{J.83}$$

J.7.5. Extended convexity for a channel. Assume a channel given by Eq. (I.76), where all the densities may depend on the parameter θ. Then the strong concavity of the Bhattacharyya coefficient described in Sec. I.7.7 implies the upper bound [79, 80]

$$F_Y(\theta) \le \mathbb{E}_\theta \left[F_{Y|X}(\theta)\right] + F_X(\theta), \tag{J.84}$$

where $F_Y(\theta)$ is the Fisher information matrix in terms of the output $f_{Y|\theta}$, $F_X(\theta)$ is the Fisher information in terms of the input $f_{X|\theta}$,

$$\mathbb{E}_\theta \left[F_{Y|X}(\theta)\right] = \int F_{Y|x}(\theta) f_{X|\theta}(x) d\sigma(x), \tag{J.85}$$

$F_{Y|x}(\theta)$ is the Fisher information in terms of the channel $f_{Y|X,\theta}$ given $X = x$, and the matrix inequality $A \le B$ means that $B - A$ is positive-semidefinite (see Sec. B.13).

J.7.6. Convexity. Following Sec. J.7.5, if the input $f_{X|\theta}$ does not depend on θ, then $F_X = 0$ and we obtain the convexity property:

$$F_Y(\theta) \le \mathbb{E}_\theta \left[F_{Y|X}(\theta)\right]. \tag{J.86}$$

J.7.7. Data-processing inequality. Following Sec. J.7.5, if the channel $f_{Y|X,\theta}$ does not depend on θ, then $F_{Y|X} = 0$ and we obtain the data-processing inequality

$$F_Y(\theta) \le F_X(\theta). \tag{J.87}$$

J.8. Proofs

We will make extensive use of the **Cauchy-Schwarz inequality (CSI)**

$$\boxed{|\langle A, B\rangle|^2 \le \langle A, A\rangle \langle B, B\rangle} \tag{J.88}$$

for an inner product. If A or B is zero, then equality holds obviously. Otherwise equality is achieved if and only if $A = cB$ for a scalar c.

PROOF OF THE GILL-LEVIT BOUND (J.20). Start with the divergence theorem, assuming $\varrho(\theta)v(\theta) = 0$ on the boundary of Θ:

$$\int \nabla \cdot [\delta(\theta)\varrho(\theta)v(\theta)]d^p\theta = 0, \tag{J.89}$$

where $\delta(\theta)$ is the bias defined by Eq. (J.59). Write

$$\nabla \cdot [\delta(\theta)\varrho(\theta)v(\theta)] = \int \nabla \cdot \left\{ \left[\check{\beta}(x) - \beta(\theta)\right] f_\theta(x)\varrho(\theta)v(\theta) \right\} d\sigma(x) \tag{J.90}$$

$$= \int \left(\check{\beta} - \beta\right) \nabla \cdot (f\varrho v) d\sigma(x) - \int (f\varrho v \cdot \nabla\beta) d\sigma(x) \tag{J.91}$$

$$= \int \left(\check{\beta} - \beta\right) \frac{\nabla \cdot (f\varrho v)}{f} f d\sigma(x) - \varrho v \cdot \nabla\beta \tag{J.92}$$

$$= \mathbb{E}_\theta \left[\left(\check{\beta} - \beta\right) \frac{\nabla \cdot (f\varrho v)}{f} \right] - \varrho v \cdot \nabla\beta, \tag{J.93}$$

so that Eq. (J.89) becomes

$$\mathbb{E}\left(v \cdot \nabla\beta\right) = \mathbb{E}\left[\left(\check{\beta} - \beta\right) \frac{\nabla \cdot (f\varrho v)}{f\varrho} \right]. \tag{J.94}$$

The CSI for the inner product $\langle A, B\rangle = \mathbb{E}(AB)$ yields

$$\left[\mathbb{E}\left(v \cdot \nabla\beta\right)\right]^2 \le \mathbb{E}\left[\left(\check{\beta} - \beta\right)^2\right] \mathbb{E}\left\{ \left[\frac{\nabla \cdot (f\varrho v)}{f\varrho} \right]^2 \right\}. \tag{J.95}$$

This is the Gill-Levit bound given by Eq. (J.20); our last task is to simplify the last term:

$$\frac{\nabla \cdot (f\varrho v)}{f\varrho} = v \cdot \nabla \ln f + \frac{1}{\varrho} \nabla \cdot (\varrho v) = v \cdot \nabla \ln f + \mathrm{div}_\varrho\, v, \tag{J.96}$$

$$\mathbb{E}\left\{ \left[\frac{\nabla \cdot (f\varrho v)}{f\varrho} \right]^2 \right\} = \mathbb{E}\left\{ (v \cdot \nabla \ln f)^2 + (\mathrm{div}_\varrho\, v)^2 + 2(\mathrm{div}_\varrho\, v) v \cdot \nabla \ln f \right\} \tag{J.97}$$

$$= \mathbb{E}\left\{ v^\top \underbrace{\mathbb{E}_\theta\left[(\nabla \ln f)\left(\nabla^\top \ln f\right) \right]}_{\equiv F \text{ by Eq. (J.24)}} v + (\mathrm{div}_\varrho\, v)^2 + 2(\mathrm{div}_\varrho\, v) v \cdot \underbrace{\mathbb{E}_\theta\left(\nabla \ln f\right)}_{=0 \text{ by Eq. (J.62)}} \right\} \tag{J.98}$$

$$= \mathbb{E}\left[v^\top F v + (\mathrm{div}_\varrho\, v)^2 \right]. \tag{J.99}$$

□

PROOF OF THE OPTIMAL GILL-LEVIT BOUND (J.28) AND (J.29). The product rule for the divergence gives

$$\nabla \cdot [(\mathrm{div}_\varrho\, v)\varrho v] = \varrho v \cdot \nabla(\mathrm{div}_\varrho\, v) + (\mathrm{div}_\varrho\, v)\nabla \cdot (\varrho v). \tag{J.100}$$

Since $\varrho v = 0$ on the boundary of Θ, $\int(\dots)d^p\theta$ of the first term vanishes, and we can write

$$\mathbb{E}\left[(\mathrm{div}_\varrho\, v)^2\right] = \int (\mathrm{div}_\varrho\, v)\nabla \cdot (\varrho v) d^p\theta = -\int \varrho v \cdot \nabla(\mathrm{div}_\varrho\, v) d^p\theta = \langle v, Dv\rangle, \tag{J.101}$$

$$Dv \equiv -\nabla(\mathrm{div}_\varrho\, v), \quad \langle v, u\rangle \equiv \int [v(\theta) \cdot u(\theta)]\varrho(\theta) d^p\theta. \tag{J.102}$$

Now the Gill-Levit bound (J.20) can be expressed as

$$G(v) = \frac{\langle v, \nabla\beta\rangle^2}{\langle v, Tv\rangle}, \tag{J.103}$$

where $T \equiv F + D$ is an operator. Notice that T is self-adjoint and positive-semidefinite, since $\langle Tv, u\rangle = \langle v, Tu\rangle$ for any u, v and the denominator of the Gill-Levit bound is nonnegative for any v. Assume, furthermore, that $\nabla\beta$ is in the range of T. Then $T^{-s}\nabla\beta$ is defined for $s > 0$, $\nabla\beta = T^s T^{-s}\nabla\beta$, and we can write

$$\langle v, \nabla\beta\rangle = \left\langle T^{1/2}v, T^{-1/2}\nabla\beta\right\rangle. \tag{J.104}$$

Now use the CSI to obtain

$$\langle v, \nabla\beta\rangle^2 \le \left\langle T^{1/2}v, T^{1/2}v\right\rangle \left\langle T^{-1/2}\nabla\beta, T^{-1/2}\nabla\beta\right\rangle = \langle v, Tv\rangle \left\langle \nabla\beta, T^{-1}\nabla\beta\right\rangle. \tag{J.105}$$

Equality is achieved if and only if

$$T^{1/2}v = cT^{-1/2}\nabla\beta, \qquad\qquad Tv = c\nabla\beta \tag{J.106}$$

for a nonzero constant c. There is no loss of generality if we set $c = 1$, and Eq. (J.28) results. Plugging the right-hand side of Eq. (J.105) into the numerator of Eq. (J.103) yields Eq. (J.29). □

Proof of Eq. (J.73). Since $\bar\beta(\theta) \equiv \mathbb{E}_\theta(\check\beta) = \mathbb{E}_\theta[\mathbb{E}_\theta(\check\beta)] = \mathbb{E}_\theta[\bar\beta(\theta)]$, $\mathbb{E}_\theta[\check\beta - \bar\beta(\theta)] = 0$, and we can write

$$v(\theta)\cdot\nabla\,\mathbb{E}_\theta\left[\check\beta - \bar\beta(\theta)\right] = v(\theta)\cdot\nabla\int\left[\check\beta(x) - \bar\beta(\theta)\right]f_\theta(x)d\sigma(x) = 0, \tag{J.107}$$

$$\int\left[v(\theta)\cdot\nabla\bar\beta(\theta)\right]f_\theta(x)d\sigma(x) = \int\left[\check\beta(x) - \bar\beta(\theta)\right][v(\theta)\cdot\nabla f_\theta(x)]d\sigma(x), \tag{J.108}$$

$$v\cdot\nabla\bar\beta = \mathbb{E}_\theta\left[\left(\check\beta - \bar\beta\right)(v\cdot\nabla\ln f)\right]. \tag{J.109}$$

The CSI in terms of $\langle A, B\rangle = \mathbb{E}_\theta(AB)$ yields

$$\left(v\cdot\nabla\bar\beta\right)^2 \le \mathbb{E}_\theta\left[\left(\check\beta - \bar\beta\right)^2\right]\mathbb{E}_\theta\left[(v\cdot\nabla\ln f)^2\right] = \mathbb{V}_\theta(\check\beta)\left(v^\top Fv\right), \tag{J.110}$$

$$\mathbb{V}_\theta(\check\beta) \ge \frac{\left(v\cdot\nabla\bar\beta\right)^2}{v^\top Fv}. \tag{J.111}$$

Now rewrite the dot product as an inner product and assume that $\nabla\beta$ is in the range of F so that $F^{-s}\nabla\beta$ is defined for $s > 0$ and $\nabla\beta = F^s F^{-s}\nabla\beta$. We obtain

$$v\cdot\nabla\bar\beta = \left\langle v, \nabla\bar\beta\right\rangle = \left\langle F^{1/2}v, F^{-1/2}\nabla\bar\beta\right\rangle. \tag{J.112}$$

Use the CSI again:

$$\left(v\cdot\nabla\bar\beta\right)^2 \le \left\langle F^{1/2}v, F^{1/2}v\right\rangle\left\langle F^{-1/2}\nabla\beta, F^{-1/2}\nabla\beta\right\rangle = \left(v^\top Fv\right)\left[(\nabla\beta)^\top F^{-1}\nabla\beta\right]. \tag{J.113}$$

Equality is achieved if and only if

$$F^{1/2}v = cF^{-1/2}\nabla\bar\beta, \qquad\qquad Fv = c\nabla\bar\beta \tag{J.114}$$

for a nonzero constant c. Plugging the right-hand side of Eq. (J.113) into the numerator of Eq. (J.111) gives Eq. (J.73). □

APPENDIX K

Solutions to Selected Problems

Exercise 3.17.

(1)

$$\left[\hat{b}_l, \hat{b}_m^\dagger\right] = \sum_s \sum_{s'} \iiint \iiint W_l^*(\boldsymbol{k}, s) W_m(\boldsymbol{k}', s') \left[\hat{a}(\boldsymbol{k}, s), \hat{a}^\dagger(\boldsymbol{k}', s')\right] d^3\boldsymbol{k} d^3\boldsymbol{k}' \tag{K.1}$$

$$= \sum_s \sum_{s'} \iiint \iiint W_l^*(\boldsymbol{k}, s) W_m(\boldsymbol{k}', s') \delta^3(\boldsymbol{k} - \boldsymbol{k}') \delta_{ss'} d^3\boldsymbol{k} d^3\boldsymbol{k}' \tag{K.2}$$

$$= \boxed{\sum_s \iiint W_l^*(\boldsymbol{k}, s) W_m(\boldsymbol{k}, s) d^3\boldsymbol{k}.} \tag{K.3}$$

(2) For $l = m$,

$$\sum_s \iiint |W_l(\boldsymbol{k}, s)|^2 d^3\boldsymbol{k} = 1. \tag{K.4}$$

Now

$$\sum_s \iiint |W_l(\boldsymbol{k}, s)|^2 d^3\boldsymbol{k} = \sum_s \delta_{s1} \int_{-\infty}^{\infty} |X(k_x)|^2 dk_x \int_{-\infty}^{\infty} |Y(k_y)|^2 dk_y \int_{-\infty}^{\infty} C^2 \,\mathrm{rect}\left(\frac{k_x - k_0}{\kappa}\right) dk_z \tag{K.5}$$

$$= \int_{k_0 - \kappa/2}^{k_0 + \kappa/2} C^2 dk_z = C^2 \kappa = 1. \tag{K.6}$$

Hence

$$\boxed{C = \frac{1}{\sqrt{\kappa}}.} \tag{K.7}$$

(3)

$$\sum_s \iiint W_l^*(\boldsymbol{k}, s) W_m(\boldsymbol{k}, s) d^3\boldsymbol{k} = \frac{1}{\kappa} \int_{k_0 - \kappa/2}^{k_0 + \kappa/2} \exp[-ik_z(z_l - z_m)] dk_z \tag{K.8}$$

$$= e^{ik_0(z_l - z_m)} \frac{\exp[-i\kappa(z_l - z_m)/2] - \exp[i\kappa(z_l - z_m)/2]}{-i\kappa(z_l - z_m)} \tag{K.9}$$

$$= e^{ik_0(z_l - z_m)} \frac{\sin[\kappa(z_l - z_m)/2]}{\kappa(z_l - z_m)/2} = e^{ik_0(z_l - z_m)} \,\mathrm{sinc}\left[\frac{\kappa}{2\pi}(z_l - z_m)\right] \tag{K.10}$$

$$= e^{ik_0(z_l - z_m)} \,\mathrm{sinc}(l - m) = \delta_{lm}. \tag{K.11}$$

(4) Eq. (3.121) is an inverse Fourier transform. The forward Fourier transform is then

$$\boxed{\hat{a}(\boldsymbol{k}, s) = \frac{1}{(2\pi)^{3/2}} \iiint \exp(-i\boldsymbol{k} \cdot \boldsymbol{r}) \hat{A}(\boldsymbol{r}, s) d^3\boldsymbol{r}.} \tag{K.12}$$

(5)

$$\left[\hat{A}(\boldsymbol{r},s),\hat{A}^\dagger(\boldsymbol{r}',s')\right]=\frac{1}{(2\pi)^3}\iiint\iiint\exp\big(i\boldsymbol{k}\cdot\boldsymbol{r}-i\boldsymbol{k}'\cdot\boldsymbol{r}'\big)[\hat{a}(\boldsymbol{k},s),\hat{a}^\dagger(\boldsymbol{k}',s')]d^3\boldsymbol{k}d^3\boldsymbol{k}' \tag{K.13}$$

$$=\frac{1}{(2\pi)^3}\iiint\iiint\exp\big(i\boldsymbol{k}\cdot\boldsymbol{r}-i\boldsymbol{k}'\cdot\boldsymbol{r}'\big)\delta^3(\boldsymbol{k}-\boldsymbol{k}')\delta_{ss'}d^3\boldsymbol{k}d^3\boldsymbol{k}' \tag{K.14}$$

$$=\delta_{ss'}\frac{1}{(2\pi)^3}\iiint\exp\big[i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')\big]d^3\boldsymbol{k} \tag{K.15}$$

$$=\boxed{\delta_{ss'}\delta^3(\boldsymbol{r}-\boldsymbol{r}').} \tag{K.16}$$

(6)

$$\hat{b}_l=\sum_s\iiint\tilde{W}_l^*(\boldsymbol{r},s)\hat{A}(\boldsymbol{r},s)d^3\boldsymbol{r}=\sum_s\iiint\tilde{W}_l^*(\boldsymbol{r},s)\left[\frac{1}{(2\pi)^{3/2}}\iiint\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\hat{a}(\boldsymbol{k},s)d^3\boldsymbol{k}\right]d^3\boldsymbol{r} \tag{K.17}$$

$$=\sum_s\iiint\left[\frac{1}{(2\pi)^{3/2}}\iiint\tilde{W}_l^*(\boldsymbol{r},s)\exp(i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{r}\right]\hat{a}(\boldsymbol{k},s)d^3\boldsymbol{k}. \tag{K.18}$$

Comparing with Eq. (3.115), we should have

$$W_l^*(\boldsymbol{k},s)=\frac{1}{(2\pi)^{3/2}}\iiint\tilde{W}_l^*(\boldsymbol{r},s)\exp(i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{r} \tag{K.19}$$

$$\boxed{W_l(\boldsymbol{k},s)=\frac{1}{(2\pi)^{3/2}}\iiint\tilde{W}_l(\boldsymbol{r},s)\exp(-i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{r},} \tag{K.20}$$

$$\boxed{\tilde{W}_l(\boldsymbol{r},s)=\frac{1}{(2\pi)^{3/2}}\iiint W_l(\boldsymbol{k},s)\exp(i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{k}.} \tag{K.21}$$

W_l and $\tilde{W}_l$ are Fourier-transform pairs.

(7) Because $\tilde{W}_l$ is the Fourier transform of W_l, we obtain

$$\tilde{W}_l(\boldsymbol{r},s)=\tilde{X}(x)\tilde{X}(y)\tilde{Z}(z), \tag{K.22}$$

$$\tilde{X}(x)\equiv\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp(ik_xx)X(k_x)dk_x, \tag{K.23}$$

$$\tilde{Y}(y)\equiv\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp(ik_yy)Y(k_y)dk_y, \tag{K.24}$$

$$\tilde{Z}_l(z)\equiv\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp(ik_zz)Z_l(k_z)dk_z \tag{K.25}$$

$$=\frac{1}{\sqrt{2\pi\kappa}}\int_{k_0-\kappa/2}^{k_0+\kappa/2}\exp[ik_z(z-z_l)]dk_z \tag{K.26}$$

$$=\frac{1}{\sqrt{2\pi\kappa}}e^{ik_0(z-z_l)}\operatorname{sinc}\left[\frac{\kappa}{2\pi}(z-z_l)\right]. \tag{K.27}$$

Exercise 3.18.

(1) It's too tedious to put hats on operators here, so I omit them.

$$\langle b:m_1,\ldots,m_J|b:n_1,\ldots,n_J\rangle$$

$$=\frac{1}{\sqrt{m_1!\ldots m_J!n_1!\ldots n_J!}}\langle\text{vac}|\,b_1^{m_1}\ldots b_J^{m_J}b_1^{\dagger n_1}\ldots b_J^{\dagger n_J}\,|\text{vac}\rangle \tag{K.28}$$

$$=\frac{1}{\sqrt{m_1!\ldots m_J!n_1!\ldots n_J!}}\langle\text{vac}|\,(b_1^{m_1}b_1^{\dagger n_1})\ldots(b_J^{m_J}b_J^{\dagger n_J})\,|\text{vac}\rangle\,.\qquad([b_j,b_l^\dagger]=0\text{ if }j\neq l) \tag{K.29}$$

We would like to simplify $b_j^{m_j} b_j^{\dagger n_j}$. Let's omit the subscripts for now, and look at $b^m b^{\dagger n}$. Actually let's look at $b b^{\dagger n}$ first. Using the commutation relation $[b, b^\dagger] = 1$, we can write

$$b b^{\dagger n} = b b^\dagger b^{\dagger n-1} = (b^\dagger b + 1) b^{\dagger n-1} = b^\dagger b b^{\dagger n-1} + b^{\dagger n-1}. \tag{K.30}$$

This is actually a recursive relation:

$$b b^{\dagger n} = b^\dagger \underbrace{b b^{\dagger n-1}}_{\text{apply Eq. (K.30)}} + b^{\dagger n-1} = b^\dagger \left(b^\dagger b b^{\dagger n-2} + b^{\dagger n-2} \right) + b^{\dagger n-1} \tag{K.31}$$

$$= b^{\dagger 2} \underbrace{b b^{\dagger n-2}}_{\text{apply Eq. (K.30)}} + 2 b^{\dagger n-1} = \dots \tag{K.32}$$

Eventually we obtain

$$b b^{\dagger n} = b^{\dagger n} b + n b^{\dagger n-1}. \tag{K.33}$$

Now we consider

$$b^n b^{\dagger n} = b^{n-1} \underbrace{b b^{\dagger n}}_{\text{apply Eq. (K.33)}} = b^{n-1} \left(b^{\dagger n} b + n b^{\dagger n-1} \right) = b^{n-1} b^{\dagger n} b + n b^{n-1} b^{\dagger n-1}. \tag{K.34}$$

This is also a recursive relation.

$$b^n b^{\dagger n} = b^{n-1} b^{\dagger n} b + n \underbrace{b^{n-1} b^{\dagger n-1}}_{\text{apply Eq. (K.34)}} = b^{n-1} b^{\dagger n} b + n \left[b^{n-2} b^{\dagger n-1} b + (n-1) \underbrace{b^{n-2} b^{\dagger n-2}}_{\text{apply Eq. (K.34)}} \right] = \dots \tag{K.35}$$

Everytime we apply Eq. (K.34), we create a new term $(\dots) b$ with the annihilation operator b at the end, plus a term $\propto b^{n-m} b^{\dagger n-m}$. Eventually we obtain

$$\boxed{b^n b^{\dagger n} = (\dots) b + n! b b^\dagger = (\dots) b + n! (b^\dagger b + 1) = (\dots) b + n!,} \tag{K.36}$$

where $(\dots)$ is a long list of terms in front of the annihilation operator b.

Remember that each b_j is a linear combination of annihilation operators $\{a_j\}$, such that

$$b_j |\text{vac}\rangle = \sum_l U_{jl} a_l |\text{vac}\rangle = 0. \tag{K.37}$$

It follows that

$$\boxed{b_j^n b_j^{\dagger n} |\text{vac}\rangle = [(\dots) b_j + n!] |\text{vac}\rangle = n! |\text{vac}\rangle .} \tag{K.38}$$

We are lucky that $b_j |\text{vac}\rangle = 0$ so we don't have to write out the terms $(\dots)$ in front of b_j.

If $m > n$, we can use similar algebra to show that

$$m > n : \qquad b^m b^{\dagger n} = (\dots) b + n! b^{m-n}, \qquad \boxed{b_j^m b_j^{\dagger n} |\text{vac}\rangle = 0.} \tag{K.39}$$

(This makes sense, since $b_j^{\dagger n}$ creates n photons in the state and b_j^m annihilates $m > n$ photons, but still we needed to prove this by algebra.) If $m < n$, we write

$$m < n : \qquad b^m b^{\dagger n} = (b^n b^{\dagger m})^\dagger, \qquad \boxed{\langle \text{vac}| b_j^m b_j^{\dagger n} = (b_j^n b_j^{\dagger m} |\text{vac}\rangle)^\dagger = 0,} \tag{K.40}$$

where the last step uses the result in Eq. (K.39). Applying these results to Eq. (K.29) gives us

$$\langle b : m_1, \dots, m_J | b : n_1, \dots, n_J \rangle = \delta_{m_1 n_1} \dots \delta_{m_J n_J}, \tag{K.41}$$

which implies that the set $\{ |b : n_1, \dots, n_J\rangle : \text{each } n_j = 0, 1, 2, \dots \}$ are orthonormal.

(2) We still have to show that the set is a basis, i.e., any $|\psi\rangle \in \mathcal{H}$ can be expressed as a linear combination of the set. We already know that $\{|a : n_1, \ldots, n_J\rangle\}$ in terms of the original modes is an orthonormal basis, so if we can prove that every normal-mode number state

$$|a : n_1, \ldots, n_J\rangle = \frac{\hat{a}_1^{\dagger n_1}}{\sqrt{n_1!}} \ldots \frac{\hat{a}_J^{\dagger n_J}}{\sqrt{n_J!}} |\text{vac}\rangle \tag{K.42}$$

can be expressed as a linear combination of the new number states $\{|b : n_1, \ldots, n_J\rangle\}$, then we are done. Recall

$$\hat{a}_j = \sum_l W_{jl} \hat{b}_l, \tag{K.43}$$

which means

$$\hat{a}_j^\dagger = \sum_l W_{jl}^* \hat{b}_l^\dagger. \tag{K.44}$$

We now prove that Eq. (K.42) is a linear combination of the new number states by induction. First note that $|\text{vac}\rangle = |b : 0, \ldots, 0\rangle$ is a new number state. If we apply one $\hat{a}_j^\dagger$ with any j to any linear combination of the new number states $\{|b : n_1, \ldots, n_J\rangle\}$, we obtain

$$\hat{a}_j^\dagger \sum_{n_1 \ldots n_J} C_{n_1 \ldots n_J} |b : n_1, \ldots, n_J\rangle = \sum_l \sum_{n_1 \ldots n_J} C_{n_1 \ldots n_J} W_{jl}^* \hat{b}_l^\dagger |b : n_1, \ldots, n_J\rangle . \tag{K.45}$$

$\hat{b}_l^\dagger |b : n_1, \ldots, n_J\rangle \propto |b : n_1, \ldots, n_l + 1, \ldots, n_J\rangle$ is proportional to a new number state, so the right-hand side of Eq. (K.45) is another linear combination of the new number states $\{|b : n_1, \ldots, n_J\rangle\}$. Hence, by induction, with the application of multiple $\hat{a}_j^\dagger$'s to $|\text{vac}\rangle$ in Eq. (K.42), the end result $|a : n_1, \ldots, n_J\rangle$ must still be a linear combination of the new number states $\{|b : n_1, \ldots, n_J\rangle\}$.

Exercise 4.17.

(1)

$$\hat{D}(\alpha) = \exp\Big(\alpha \hat{a}^\dagger - \alpha^* \hat{a}\Big) = \exp\Big[\alpha(\hat{q} - i\hat{p})/\sqrt{2} - \alpha^*(\hat{q} + i\hat{p})/\sqrt{2}\Big] \tag{K.46}$$

$$= \exp\Big\{i[(\alpha - \alpha^*)/(\sqrt{2}i)]\hat{q} - i[(\alpha + \alpha^*)/\sqrt{2}]\hat{p}\Big\}. \tag{K.47}$$

Hence

$$\boxed{\xi = \frac{1}{\sqrt{2}i}(\alpha - \alpha^*) = \sqrt{2}\,\text{Im}\,\alpha,} \qquad \boxed{\eta = \frac{1}{\sqrt{2}}(\alpha + \alpha^*) = \sqrt{2}\,\text{Re}\,\alpha.} \tag{K.48}$$

(2) BCH formula:

$$(\exp \hat{A})(\exp \hat{B}) = \exp\left(\hat{A} + \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{12}[\hat{A}, [\hat{A}, \hat{B}]] - \frac{1}{12}[\hat{B}, [\hat{A}, \hat{B}]] + \ldots\right). \tag{K.49}$$

Let

$$\hat{A} = i\xi\hat{q}, \quad \hat{B} = -i\eta\hat{p}, \tag{K.50}$$

$$[\hat{A}, \hat{B}] = \xi\eta[\hat{q}, \hat{p}] = i\xi\eta, \tag{K.51}$$

$$\exp(i\xi\hat{q}) \exp(-i\eta\hat{p}) = \exp(i\xi\hat{q} - i\eta\hat{p} + i\xi\eta). \tag{K.52}$$

Similarly,

$$\hat{A} = -i\eta\hat{p}, \quad \hat{B} = i\xi\hat{q}, \tag{K.53}$$

$$[\hat{A}, \hat{B}] = \xi\eta[\hat{p}, \hat{q}] = -i\xi\eta, \tag{K.54}$$

$$\exp(-i\eta\hat{p}) \exp(i\xi\hat{q}) = \exp(i\xi\hat{q} - i\eta\hat{p} - i\xi\eta). \tag{K.55}$$

Hence

$$\boxed{\exp(i\xi\hat{q} - i\eta\hat{p}) = \exp(-i\xi\eta)\exp(i\xi\hat{q})\exp(-i\eta\hat{p}) = \exp(i\xi\eta)\exp(-i\eta\hat{p})\exp(i\xi\hat{q}).} \tag{K.56}$$

(3)

$$\hat{D}(\alpha)\,|q=x\rangle = e^{i\xi\hat{q}-i\eta\hat{p}}\,|q=x\rangle \tag{K.57}$$

$$= e^{i\xi\eta}e^{-i\eta\hat{p}}e^{i\xi\hat{q}}\,|q=x\rangle \qquad \text{(using previous results)} \tag{K.58}$$

$$= e^{i\xi\eta}e^{-i\eta\hat{p}}e^{i\xi x}\,|q=x\rangle \qquad (|q=x\rangle \text{ is eigenstate of } e^{i\xi\hat{q}}) \tag{K.59}$$

$$= e^{i\xi\eta}e^{-i\eta\hat{p}}e^{i\xi x}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-iyx}\,|p=y\rangle\,dy \qquad \text{(write } |q=x\rangle \text{ in terms of } \{|p=y\rangle\}) \tag{K.60}$$

$$= e^{i\xi(x+\eta)}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-i\eta y}e^{-iyx}\,|p=y\rangle\,dy \qquad (|p=y\rangle \text{ is eigenstate of } e^{-i\eta\hat{p}}) \tag{K.61}$$

$$= e^{i\xi(x+\eta)}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-iy(x+\eta)}\,|p=y\rangle\,dy \tag{K.62}$$

$$= \boxed{e^{i\xi(x+\eta)}\,|q=x+\eta\rangle\,,} \tag{K.63}$$

where ξ and η are given by Eqs. (K.48). The phase factor $e^{i\xi(x+\eta)}$ is not very important. The important point is that $\hat{D}(\alpha)$ shifts the $|q=x\rangle$ state to the $|q=x+\eta\rangle$ state with a new eigenvalue $x+\eta$, where $\eta = \sqrt{2}\,\mathrm{Re}\,\alpha$ is the displacement. Similarly,

$$\hat{D}(\alpha)\,|p=y\rangle = e^{-i\xi\eta}e^{i\xi\hat{q}}e^{-i\eta\hat{p}}\,|p=y\rangle = e^{-i\xi\eta}e^{i\xi\hat{q}}e^{-i\eta y}\,|p=y\rangle \tag{K.64}$$

$$= e^{-i\xi\eta}e^{i\xi\hat{q}}e^{-i\eta y}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{iyx}\,|q=x\rangle\,dx \tag{K.65}$$

$$= e^{-i\xi\eta}e^{-i\eta y}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i(y+\xi)x}\,|q=x\rangle\,dx \tag{K.66}$$

$$= \boxed{e^{-i\eta(y+\xi)}\,|p=y+\xi\rangle\,.} \tag{K.67}$$

(4) To verify Eq. (4.6), write

$$\langle n|\alpha\rangle = \langle n|\,e^{-|\alpha|^2/2}\sum_{m=0}^{\infty}\frac{\alpha^m}{\sqrt{m!}}\,|m\rangle \qquad \text{(definition of } |\alpha\rangle) \tag{K.68}$$

$$= e^{-|\alpha|^2/2}\frac{\alpha^n}{\sqrt{n!}}. \qquad (\langle n|m\rangle = \delta_{nm}) \tag{K.69}$$

Then

$$\boxed{|\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2}\frac{|\alpha|^{2n}}{n!}.} \tag{K.70}$$

To verify Eq. (4.7), consider

$$\langle q=x|\alpha\rangle = \langle q=x|\,\hat{D}(\alpha)\,|0\rangle = (\hat{D}^\dagger(\alpha)\,|q=x\rangle)^\dagger\,|0\rangle = (\hat{D}(-\alpha)\,|q=x\rangle)^\dagger\,|0\rangle\,. \tag{K.71}$$

Now use the previous result to obtain

$$\hat{D}(-\alpha)\,|q=x\rangle = e^{i\theta}\left|q=x-\sqrt{2}\,\mathrm{Re}\,\alpha\right\rangle, \tag{K.72}$$

where θ is an unimportant phase. Hence

$$\langle q = x|\alpha\rangle = e^{-i\theta}\left\langle q = x - \sqrt{2}\,\mathrm{Re}\,\alpha\middle|0\right\rangle \tag{K.73}$$

$$= e^{-i\theta}\frac{1}{\pi^{1/4}}\exp\left[-\frac{1}{2}\left(x - \sqrt{2}\,\mathrm{Re}\,\alpha\right)^2\right], \qquad \text{(using Eq. (4.1))} \tag{K.74}$$

$$\boxed{|\langle q = x|\alpha\rangle|^2 = \frac{1}{\sqrt{\pi}}\exp\left[-\left(x - \sqrt{2}\,\mathrm{Re}\,\alpha\right)^2\right].} \tag{K.75}$$

The derivation of Eq. (4.8) is similar.

Exercise 4.26.

(1) This is very similar to the Heisenberg picture of $\hat{a}$. The trick is to do a $\partial/\partial\theta$:

$$\frac{\partial\hat{a}(\theta)}{\partial\theta} = i\hat{n}\hat{R}^\dagger(\theta)\hat{a}\hat{R}(\theta) - i\hat{R}^\dagger(\theta)\hat{a}\hat{R}(\theta)\hat{n} = -i\hat{R}^\dagger(\theta)[\hat{a},\hat{n}]\hat{R}(\theta) = -i\hat{a}(\theta). \tag{K.76}$$

This differential equation has the solution

$$\boxed{\hat{a}(\theta) = \hat{a}\exp(-i\theta).} \tag{K.77}$$

It follows that

$$\hat{a}^\dagger(\theta) = \hat{R}^\dagger(\theta)\hat{a}^\dagger\hat{R}(\theta) = \left[\hat{R}^\dagger(\theta)\hat{a}\hat{R}(\theta)\right]^\dagger = \hat{a}^\dagger\exp(i\theta), \tag{K.78}$$

$$\hat{q}(\theta) = \frac{1}{\sqrt{2}}\hat{R}^\dagger(\theta)(\hat{a} + \hat{a}^\dagger)\hat{R}(\theta) = \boxed{\frac{1}{\sqrt{2}}\left[\hat{a}\exp(-i\theta) + \hat{a}^\dagger\exp(i\theta)\right],} \tag{K.79}$$

$$\hat{p}(\theta) = \boxed{\frac{1}{\sqrt{2}i}\left[\hat{a}\exp(-i\theta) - \hat{a}^\dagger\exp(i\theta)\right].} \tag{K.80}$$

(2)

$$\hat{q}(\theta)\hat{R}^\dagger(\theta)\,|q = x\rangle = \hat{R}^\dagger(\theta)\hat{q}\hat{R}(\theta)\hat{R}^\dagger(\theta)\,|q = x\rangle \tag{K.81}$$

$$= \hat{R}^\dagger(\theta)\hat{q}\,|q = x\rangle \qquad (\hat{R}\text{ is unitary}) \tag{K.82}$$

$$= \hat{R}^\dagger(\theta)x\,|q = x\rangle = x\hat{R}^\dagger(\theta)\,|q = x\rangle\,. \tag{K.83}$$

Similarly,

$$\hat{p}(\theta)\hat{R}^\dagger(\theta)\,|p = y\rangle = \hat{R}^\dagger(\theta)\hat{p}\hat{R}(\theta)\hat{R}^\dagger(\theta)\,|p = y\rangle \tag{K.84}$$

$$= \hat{R}^\dagger(\theta)\hat{p}\,|p = y\rangle = \hat{R}^\dagger(\theta)y\,|p = y\rangle = y\hat{R}^\dagger(\theta)\,|p = y\rangle\,. \tag{K.85}$$

(3)

$$\left\langle q(\theta) = x\middle|q(\theta) = x'\right\rangle = \langle q = x|\,\hat{R}(\theta)\hat{R}^\dagger(\theta)\,\left|q = x'\right\rangle \qquad \text{(by definition of } |q(\theta) = x\rangle) \tag{K.86}$$

$$= \left\langle q = x\middle|q = x'\right\rangle \qquad (\hat{R}\text{ is unitary}) \tag{K.87}$$

$$= \delta(x - x'). \qquad \text{(Eq. (3.22))} \tag{K.88}$$

$$\int_{-\infty}^{\infty} |q(\theta)=x\rangle \langle q(\theta)=x| \, dx$$

$$= \int_{-\infty}^{\infty} \hat{R}^\dagger(\theta) |q=x\rangle \langle q=x| \hat{R}(\theta) dx \qquad \text{(by definition of } |q(\theta)=x\rangle) \tag{K.89}$$

$$= \hat{R}^\dagger(\theta) \left[\int_{-\infty}^{\infty} |q=x\rangle \langle q=x| \, dx \right] \hat{R}(\theta) \qquad \text{(operators are linear)} \tag{K.90}$$

$$= \hat{R}^\dagger(\theta) \hat{I} \hat{R}(\theta) \qquad \text{(Eq. (3.24))} \tag{K.91}$$

$$= \hat{R}^\dagger(\theta) \hat{R}(\theta) = \hat{I}. \qquad (\hat{R} \text{ is unitary}) \tag{K.92}$$

The derivation for the $\hat{p}(\theta)$ eigenstates is similar.

(4) From previous results, we can write

$$\hat{q}(\theta)\hat{I} = \hat{q} \int_{-\infty}^{\infty} |q(\theta)=x\rangle \langle q(\theta)=x| \, dx = \int_{-\infty}^{\infty} \hat{q} \, |q(\theta)=x\rangle \langle q(\theta)=x| \, dx \tag{K.93}$$

$$= \int_{-\infty}^{\infty} x \, |q(\theta)=x\rangle \langle q(\theta)=x| \, dx. \tag{K.94}$$

The diagonal form of $\hat{p}(\theta)$ can be derived similarly.

(5)

$$\hat{R}(\theta) |\alpha\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\hat{n}\theta} |n\rangle \tag{K.95}$$

$$= \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-in\theta} |n\rangle = \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\theta})^n}{\sqrt{n!}} |n\rangle = \boxed{\left|\alpha e^{-i\theta}\right\rangle}. \tag{K.96}$$

(6)

$$|\langle q(\theta)=x|\alpha\rangle|^2 = \left|\langle q=x| \hat{R}(\theta) |\alpha\rangle\right|^2 = \left|\left\langle q=x\middle|\alpha e^{-i\theta}\right\rangle\right|^2 \tag{K.97}$$

$$= \boxed{\frac{1}{\sqrt{\pi}} \exp\left\{ -\left[x - \sqrt{2}\,\mathrm{Re}(\alpha e^{-i\theta}) \right]^2 \right\}}. \tag{K.98}$$

Similarly,

$$|\langle p(\theta)=y|\alpha\rangle|^2 = \left|\langle p=y| \hat{R}(\theta) |\alpha\rangle\right|^2 = \left|\left\langle p=y\middle|\alpha e^{-i\theta}\right\rangle\right|^2 \tag{K.99}$$

$$= \boxed{\frac{1}{\sqrt{\pi}} \exp\left\{ -\left[y - \sqrt{2}\,\mathrm{Im}(\alpha e^{-i\theta}) \right]^2 \right\}}. \tag{K.100}$$

(7) Use Glauber's formula:

$$\langle q(\theta)=x| \hat{\rho} |q(\theta)=x\rangle = \iint \Phi(\alpha) |\langle q(\theta)=x|\alpha\rangle|^2 d^2\alpha. \tag{K.101}$$

Let

$$u \equiv \sqrt{2}\,\mathrm{Re}(\alpha e^{-i\theta}), \qquad v \equiv \sqrt{2}\,\mathrm{Im}(\alpha e^{-i\theta}). \tag{K.102}$$

Convince yourself that

$$du\,dv = 2(d\,\mathrm{Re}\,\alpha)(d\,\mathrm{Im}\,\alpha), \qquad d^2\alpha \equiv (d\,\mathrm{Re}\,\alpha)(d\,\mathrm{Im}\,\alpha) = \frac{1}{2} du\,dv. \tag{K.103}$$

In terms of the new variables,

$$\Phi(\alpha) = \frac{1}{\pi\bar{n}} \exp\left(-\frac{|\alpha|^2}{\bar{n}}\right) = \frac{1}{\pi\bar{n}} \exp\left(-\frac{u^2+v^2}{2\bar{n}}\right), \tag{K.104}$$

$$|\langle q(\theta) = x|\alpha\rangle|^2 = \frac{1}{\sqrt{\pi}} \exp\left\{-\left[x - \sqrt{2}\,\mathrm{Re}(\alpha e^{-i\theta})\right]^2\right\} = \frac{1}{\sqrt{\pi}} \exp\left[-(x-u)^2\right]. \tag{K.105}$$

Hence

$$\langle q(\theta) = x|\,\hat{\rho}\,|q(\theta) = x\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1}{2\pi\bar{n}} \exp\left(-\frac{u^2+v^2}{2\bar{n}}\right) \frac{1}{\sqrt{\pi}} \exp\left[-(x-u)^2\right] du dv \tag{K.106}$$

$$= \left[\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\bar{n}}} \exp\left(-\frac{v^2}{2\bar{n}}\right) dv\right] \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\bar{n}}} \exp\left(-\frac{u^2}{2\bar{n}}\right) \frac{1}{\sqrt{\pi}} \exp\left[-(x-u)^2\right] du \tag{K.107}$$

$$= \boxed{\frac{1}{\sqrt{2\pi(\bar{n}+1/2)}} \exp\left[-\frac{x^2}{2(\bar{n}+1/2)}\right].} \tag{K.108}$$

This is a Gaussian distribution with zero mean and variance equal to $\bar{n} + 1/2$. Similarly,

$$\langle p(\theta) = y|\,\hat{\rho}\,|p(\theta) = y\rangle = \boxed{\frac{1}{\sqrt{2\pi(\bar{n}+1/2)}} \exp\left[-\frac{y^2}{2(\bar{n}+1/2)}\right].} \tag{K.109}$$

Exercise 4.28. Let the photon-number random variable be n. Let α be another random variable with probability density $\Phi(\alpha)$. The probability mass function of n is

$$P(n) = \iint \Phi(\alpha)|\,\langle n|\alpha\rangle\,|^2 d^2\alpha. \tag{K.110}$$

This formula is consistent with probability theory if we regard

$$P(n|\alpha) = |\,\langle n|\alpha\rangle\,|^2 \tag{K.111}$$

as the probability mass function of n conditioned on a value of α. By the law of total variance, the variance of n is given by

$$\mathbb{V}(n) = \mathbb{E}[\mathbb{V}(n|\alpha)] + \mathbb{V}[\mathbb{E}(n|\alpha)]. \tag{K.112}$$

$P(n|\alpha)$ is Poisson, so we know that

$$\mathbb{E}(n|\alpha) = |\alpha|^2, \qquad \mathbb{V}(n|\alpha) = |\alpha|^2. \tag{K.113}$$

It follows that

$$\mathbb{V}(n) = \mathbb{E}\left(|\alpha|^2\right) + \mathbb{V}\left(|\alpha|^2\right), \tag{K.114}$$

where $\mathbb{E}(|\alpha|^2)$ and $\mathbb{V}(|\alpha|^2)$ can be computed using Φ as the probability density. Now notice that the mean photon number is given by

$$\bar{n} = \sum_n nP(n) = \iint \Phi(\alpha) \sum_n n|\,\langle n|\alpha\rangle\,|^2 d^2\alpha = \iint \Phi(\alpha)|\alpha|^2 d^2\alpha = \mathbb{E}\left(|\alpha|^2\right). \tag{K.115}$$

Hence

$$\mathbb{V}(n) = \bar{n} + \mathbb{V}\left(|\alpha|^2\right). \tag{K.116}$$

The variance of a random variable is always nonnegative, so $\mathbb{V}(|\alpha|^2) \geq 0$, and we must have $\mathbb{V}(n) \geq \bar{n}$.

Exercise 6.5. We know that, for normal modes,

$$\hat{a}_j(t) = \hat{a}_j \exp(-i\omega_j t), \tag{K.117}$$

so the $V(t)$ matrix is simply the diagonal matrix:

$$\boxed{V_{jl}(t) = \delta_{jl} \exp(-i\omega_j t).} \tag{K.118}$$

Exercise 6.8. Given Eqs. (6.65) and (K.118), the amplitude of the coherent state $|V(t)\boldsymbol{\alpha}\rangle$ at time t is simply

$$\alpha_j(t) = \alpha_j \exp(-i\omega_j t) \propto \delta_{s1}\delta_{k_x 0}\delta_{k_y 0} g(k_z) \exp(-ik_z z_1) \exp(-i\omega_j t). \tag{K.119}$$

Remember that $\omega_j = c|\boldsymbol{k}|$. $\alpha_j(t)$ is nonzero only when $k_x = 0$, $k_y = 0$, and $k_z \geq 0$. We can then assume

$$\omega_j = c|\boldsymbol{k}| = c|k_z| = ck_z. \tag{K.120}$$

Hence

$$\alpha_j(t) \propto \delta_{s1}\delta_{k_x 0}\delta_{k_y 0} g(k_z) \exp(-ik_z z_0) \exp(-ick_z t) \tag{K.121}$$

$$= \delta_{s1}\delta_{k_x 0}\delta_{k_y 0} g(k_z) \exp[-ik_z(z_1 + ct)]. \tag{K.122}$$

This $(\boldsymbol{k}, s)$-space amplitude corresponds to a pulse with center at $z_1 + ct$.

Exercise 6.10.

(1) A unitary V satisfies $VV^\dagger = I$. In the index notation,

$$\sum_j V_{lj} V^*_{mj} = \delta_{lm}, \tag{K.123}$$

which implies

$$\sum_j V_{3j} V^*_{3j} = \sum_j |V_{3j}|^2 = |V_{31}|^2 + |V_{32}|^2 + \cdots = 1, \tag{K.124}$$

$$\sum_j V_{4j} V^*_{4j} = \sum_j |V_{4j}|^2 = |V_{41}|^2 + |V_{42}|^2 + \cdots = 1, \tag{K.125}$$

$$\sum_j V_{3j} V^*_{4j} = V_{31} V^*_{41} + V_{32} V^*_{42} + \cdots = 0. \tag{K.126}$$

If we assume Eq. (6.85), then

$$|V_{31}|^2 + |V_{32}|^2 = 1, \qquad |V_{41}|^2 + |V_{42}|^2 = 1, \qquad V_{31} V^*_{41} + V_{32} V^*_{42} = 0. \tag{K.127}$$

These equations imply that

$$SS^\dagger = \begin{pmatrix} V_{31} & V_{32} \\ V_{41} & V_{42} \end{pmatrix} \begin{pmatrix} V^*_{31} & V^*_{41} \\ V^*_{32} & V^*_{42} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \tag{K.128}$$

so $S^\dagger = S^{-1}$, meaning that S is unitary.

Conversely, if S is unitary, $SS^\dagger = I$, and we have

$$|V_{31}|^2 + |V_{32}|^2 = 1, \qquad |V_{41}|^2 + |V_{42}|^2 = 1, \qquad V_{31} V^*_{41} + V_{32} V^*_{42} = 0. \tag{K.129}$$

Plug these into Eqs. (K.124) and (K.125) to obtain

$$\sum_j |V_{3j}|^2 = |V_{31}|^2 + |V_{32}|^2 + \sum_{j=3}^{J} |V_{3j}|^2 = 1 + \sum_{j=3}^{J} |V_{3j}|^2 = 1, \qquad \sum_{j=3}^{J} |V_{3j}|^2 = 0, \tag{K.130}$$

$$\sum_j |V_{4j}|^2 = |V_{41}|^2 + |V_{42}|^2 + \sum_{j=3}^{J} |V_{4j}|^2 = 1 + \sum_{j=3}^{J} |V_{4j}|^2 = 1, \qquad \sum_{j=3}^{J} |V_{4j}|^2 = 0. \tag{K.131}$$

A sum of nonnegative numbers is equal to 0 if and only if all the numbers are zero. Hence

$$|V_{3j}|^2 = 0 \text{ and } |V_{4j}|^2 = 0, \quad j = 3, 4, \ldots, \tag{K.132}$$

which implies Eq. (6.85).

(2) A unitary V also satisfies $V^\dagger V = I$. Then

$$\sum_j V_{jl}^* V_{jm} = \delta_{lm}, \tag{K.133}$$

$$\sum_j |V_{j1}|^2 = |V_{31}|^2 + |V_{41}|^2 + \sum_{j\neq 3 \text{ and } j\neq 4} |V_{j1}|^2 = 1, \tag{K.134}$$

$$\sum_j |V_{j2}|^2 = |V_{32}|^2 + |V_{42}|^2 + \sum_{j\neq 3 \text{ and } j\neq 4} |V_{j2}|^2 = 1, \tag{K.135}$$

$$\sum_j V_{j1}^* V_{j2} = V_{31}^* V_{32} + V_{41}^* V_{42} + \sum_{j\neq 3 \text{ and } j\neq 4} V_{j1}^* V_{j2} = 0. \tag{K.136}$$

Eq. (6.88) implies that all the $\sum_{j\neq 3 \text{ and } j\neq 4}(\ldots)$ terms above are zero, leading to

$$|V_{31}|^2 + |V_{41}|^2 = 1, \qquad |V_{32}|^2 + |V_{42}|^2 = 1, \qquad V_{31}^* V_{32} + V_{41}^* V_{42} = 0. \tag{K.137}$$

These equations imply that $S^\dagger S = I$, which implies $S^\dagger = S^{-1}$, meaning that S is unitary. The converse is very similar to the converse proof in part (1).

Exercise 6.11. One trick is to write

$$\hat{a}_3^\dagger(T)\hat{a}_3(T) + \hat{a}_4^\dagger(T)\hat{a}_4(T) = \begin{pmatrix}\hat{a}_3^\dagger(T) & \hat{a}_4^\dagger(T)\end{pmatrix}\begin{pmatrix}\hat{a}_3(T)\\ \hat{a}_4(T)\end{pmatrix}, \tag{K.138}$$

$$\begin{pmatrix}\hat{a}_3(T)\\ \hat{a}_4(T)\end{pmatrix} = S\begin{pmatrix}\hat{a}_1(0)\\ \hat{a}_2(0)\end{pmatrix}, \tag{K.139}$$

$$\begin{pmatrix}\hat{a}_3^\dagger(T) & \hat{a}_4^\dagger(T)\end{pmatrix} = \begin{pmatrix}\hat{a}_1^\dagger(0) & \hat{a}_2^\dagger(0)\end{pmatrix}S^\dagger, \tag{K.140}$$

so that

$$\hat{a}_3^\dagger(T)\hat{a}_3(T) + \hat{a}_4^\dagger(T)\hat{a}_4(T) = \begin{pmatrix}\hat{a}_1^\dagger(0) & \hat{a}_2^\dagger(0)\end{pmatrix}S^\dagger S\begin{pmatrix}\hat{a}_1(0)\\ \hat{a}_2(0)\end{pmatrix} = \begin{pmatrix}\hat{a}_1^\dagger(0) & \hat{a}_2^\dagger(0)\end{pmatrix}\begin{pmatrix}\hat{a}_1(0)\\ \hat{a}_2(0)\end{pmatrix} \tag{K.141}$$

$$= \hat{a}_1^\dagger(0)\hat{a}_1(0) + \hat{a}_2^\dagger(0)\hat{a}_2(0). \tag{K.142}$$

Exercise 6.13. Consider the J-input-J-output relation

$$\alpha_j(T) = \sum_l V_{jl}\alpha_l(0). \tag{K.143}$$

Since V is unitary, we have this energy conservation:

$$\sum_j |\alpha_j(T)|^2 = \sum_{j,l,m} V_{jl}^* V_{jm}\alpha_l^*(0)\alpha_m(0) = \sum_{l,m}\delta_{lm}\alpha_l^*(0)\alpha_m(0) \tag{K.144}$$

$$= \sum_l |\alpha_l(0)|^2. \tag{K.145}$$

Now let's set all the input amplitudes $\alpha_l(0)$ to be zero for all l except mode 1 and 2. Then energy conservation implies

$$\sum_j |\alpha_j(T)|^2 = |\alpha_1(0)|^2 + |\alpha_2(0)|^2. \tag{K.146}$$

We also know that the output energy in mode 3 and 4 must be smaller than the total output:

$$|\alpha_3(T)|^2 + |\alpha_4(T)|^2 \leq \sum_j |\alpha_j(T)|^2. \tag{K.147}$$

Hence

$$|\alpha_3(T)|^2 + |\alpha_4(T)|^2 \leq |\alpha_1(0)|^2 + |\alpha_2(0)|^2. \tag{K.148}$$

Exercise 8.2.

(1) Because the state $|\psi\rangle \otimes |\alpha_2\rangle$ for the two input modes is a tensor product, the average of a product of any two operators $\hat{A}_1$ and $\hat{A}_2$, where $\hat{A}_1$ is an operator for the first mode and $\hat{A}_2$ is an operator for the second mode, can be factorized as

$$\left\langle \hat{A}_1\hat{A}_2 \right\rangle = \left\langle \hat{A}_1 \otimes \hat{A}_2 \right\rangle = \langle\psi| \otimes \langle\alpha_2| \hat{A}_1 \otimes \hat{A}_2 |\psi\rangle \otimes |\alpha_2\rangle = \langle\psi| \otimes \langle\alpha_2| \left(\hat{A}_1 |\psi\rangle \otimes \hat{A}_2 |\alpha_2\rangle\right) \tag{K.149}$$

$$= \langle\psi| \hat{A}_1 |\psi\rangle \langle\alpha_2| \hat{A}_2 |\alpha_2\rangle = \left\langle \hat{A}_1 \right\rangle \left\langle \hat{A}_2 \right\rangle. \tag{K.150}$$

Then

$$\langle O\rangle = e^{i\theta} \left\langle \hat{a}_1^\dagger \hat{a}_2 \right\rangle + e^{-i\theta} \left\langle \hat{a}_1 \hat{a}_2^\dagger \right\rangle = e^{i\theta} \left\langle \hat{a}_1^\dagger \right\rangle \langle \hat{a}_2\rangle + e^{-i\theta} \langle a_1\rangle \left\langle \hat{a}_2^\dagger \right\rangle = e^{i\theta}\alpha_2 \langle \hat{a}_1\rangle^* + \text{c.c.}, \tag{K.151}$$

$$\left\langle O'\right\rangle = e^{i\theta} \left\langle \alpha_2 \hat{a}_1^\dagger \right\rangle + e^{-i\theta} \langle \hat{a}_1 \alpha_2^*\rangle = e^{i\theta}\alpha_2 \left\langle \hat{a}_1^\dagger \right\rangle + \text{c.c.} = \langle O\rangle. \tag{K.152}$$

(2) Let's compute $\left\langle O^2\right\rangle$ and $\left\langle O'^2\right\rangle$ first.

$$\left\langle O^2\right\rangle = e^{i\theta} \left\langle \hat{a}_1^{\dagger 2} \right\rangle \langle \hat{a}_2^2\rangle + \text{c.c.} + \left\langle \hat{a}_1^\dagger \hat{a}_1 \right\rangle \left\langle \hat{a}_2 \hat{a}_2^\dagger \right\rangle + \left\langle \hat{a}_1 \hat{a}_1^\dagger \right\rangle \left\langle \hat{a}_2^\dagger \hat{a}_2 \right\rangle \tag{K.153}$$

$$= e^{i\theta}\alpha_2^2 \left\langle \hat{a}_1^{\dagger 2} \right\rangle + \text{c.c.} + \left(|\alpha_2|^2 + 1\right) \left\langle \hat{a}_1^\dagger \hat{a}_1 \right\rangle + |\alpha_2|^2 \left\langle \hat{a}_1 \hat{a}_1^\dagger \right\rangle, \tag{K.154}$$

$$\left\langle O'^2\right\rangle = e^{i\theta}\alpha_2^2 \left\langle \hat{a}_1^{\dagger 2} \right\rangle + \text{c.c.} + |\alpha_2|^2 \left\langle \hat{a}_1^\dagger \hat{a}_1 \right\rangle + |\alpha_2|^2 \left\langle \hat{a}_1 \hat{a}_1^\dagger \right\rangle. \tag{K.155}$$

So

$$\left\langle O^2\right\rangle = \left\langle O'^2\right\rangle + \left\langle \hat{a}_1^\dagger \hat{a}_1 \right\rangle. \tag{K.156}$$

Now the variances are given by

$$\left\langle \Delta O^2\right\rangle = \left\langle O^2\right\rangle - \langle O\rangle^2 = \left\langle O'^2\right\rangle + \left\langle \hat{a}_1^\dagger \hat{a}_1 \right\rangle - \left\langle O'\right\rangle^2 = \left\langle \Delta O'^2\right\rangle + \left\langle \hat{a}_1^\dagger \hat{a}_1 \right\rangle. \tag{K.157}$$

(3) Let a normalized quadrature operator be

$$\hat{q} \equiv \frac{1}{\sqrt{2}} \left(e^{i\theta + \angle\alpha_2} \hat{a}_1^\dagger + \text{H.c.}\right), \qquad \hat{O}' = \sqrt{2}|\alpha_2|\hat{q}. \tag{K.158}$$

If the first input is a coherent state $|\alpha\rangle$,

$$\langle \hat{a}_1^\dagger \hat{a}_1\rangle = |\alpha|^2, \tag{K.159}$$

$$\left\langle \Delta O'^2\right\rangle = 2|\alpha_2|^2 \left\langle \Delta q^2\right\rangle = |\alpha_2|^2. \tag{K.160}$$

It follows that the difference between $\left\langle \Delta O^2\right\rangle$ and $\left\langle \Delta O'^2\right\rangle$ is negligible when

$$\langle \hat{a}_1^\dagger \hat{a}_1\rangle = |\alpha|^2 \ll \left\langle \Delta O'^2\right\rangle = |\alpha_2|^2. \tag{K.161}$$

Exercise 8.7.

(1)

$$\bar{X}_m = \sqrt{\frac{2}{M}}\,\mathrm{Re}\left((\mathrm{Re}\,\alpha + i\,\mathrm{Im}\,\alpha)(\cos\phi_m - i\sin\phi_m)\right) \tag{K.162}$$

$$= \sqrt{\frac{2}{M}}\,\mathrm{Re}\left((\mathrm{Re}\,\alpha)\cos\phi_m + (\mathrm{Im}\,\alpha)\sin\phi_m + i(\dots)\right) = \sqrt{\frac{2}{M}}(\mathrm{Re}\,\alpha)\cos\phi_m + (\mathrm{Im}\,\alpha)\sin\phi_m. \tag{K.163}$$

(2)

$$\sum_{m=0}^{M-1}\cos^2\phi_m = \sum_{m=0}^{M-1}\frac{1+\cos(2\phi_m)}{2} = \frac{M}{2} + \frac{1}{4}\left(\sum_{m=0}^{M-1} e^{i2\phi_m} + \text{c.c.}\right). \tag{K.164}$$

Now we evaluate the sum of complex exponentials:

$$\sum_{m=0}^{M-1} e^{i2\phi_m} = \sum_{m=0}^{M-1} e^{i2(\phi_0-\Omega t_m)} = e^{i2\phi_0}\sum_{m=0}^{M-1} e^{-i2\pi Lm/M} = e^{i2\phi_0}\frac{1-e^{-i2\pi L}}{1-e^{-i2\pi L/M}}, \tag{K.165}$$

where the last step comes from the geometric series (https://en.wikipedia.org/wiki/Geometric_series). Since L is an integer, $e^{-i2\pi L} = 1$, the numerator is zero. With $|L| < M$, $e^{-i2\pi L/M}$ is not equal to 1, so the denominator is not zero. Eq. (K.165) is then zero, c.c. in Eq. (K.164) is also zero, and we arrive at $M/2$ for Eq. (K.164).

The other identities are similar:

$$\sum_{m=0}^{M-1}\sin^2\phi_m = \sum_{m=0}^{M-1}\left(1-\cos^2\phi_m\right) = M - \sum_{m=0}^{M-1}\cos^2\phi_m = M - \frac{M}{2} = \frac{M}{2}. \tag{K.166}$$

$$\sum_{m=0}^{M-1}\sin\phi_m\cos\phi_m = \frac{1}{2}\sum_{m=0}^{M-1}\sin(2\phi_m) = \frac{1}{2}\sum_{m=0}^{M-1}\sin(2\phi_m) = \frac{1}{4i}\sum_{m=0}^{M-1}(e^{i2\phi_m} - \text{c.c.}) = 0. \tag{K.167}$$

(3) Y_1 and Y_2 are linear combinations of Gaussian random variables, so they are also Gaussian random variables. Now we can use the previous results to compute their expected values:

$$\mathbb{E}(Y_1) = \sqrt{\frac{2}{M}}\sum_m \mathbb{E}(X_m)\cos\phi_m = \frac{2}{M}\sum_m\left(\mathrm{Re}\,\alpha\cos\phi_m + \mathrm{Im}\,\alpha\sin\phi_m\right)\cos\phi_m \tag{K.168}$$

$$= \frac{2}{M}\sum_m\left(\mathrm{Re}\,\alpha\cos^2\phi_m + \mathrm{Im}\,\alpha\sin\phi_m\cos\phi_m\right) \tag{K.169}$$

$$= \frac{2}{M}\left(\mathrm{Re}\,\alpha\sum_m\cos^2\phi_m + \mathrm{Im}\,\alpha\sum_m\sin\phi_m\cos\phi_m\right) = \mathrm{Re}\,\alpha. \tag{K.170}$$

$\mathbb{E}(Y_2)$ is similar. To compute the variance of Y_1, we can subtract its mean first:

$$Y_1 - \mathbb{E}(Y_1) = \sqrt{\frac{2}{M}} \sum_m Z_m \cos\phi_m, \tag{K.171}$$

$$\mathbb{V}(Y_1) = \mathbb{E}\left\{[Y_1 - \mathbb{E}(Y_1)]^2\right\} = \mathbb{E}\left\{\left[\sqrt{\frac{2}{M}} \sum_m Z_m \cos\phi_m\right]^2\right\} \tag{K.172}$$

$$= \frac{2}{M}\,\mathbb{E}\left\{\sum_{m,l} Z_m Z_l \cos\phi_m \cos\phi_l\right\} = \frac{2}{M}\sum_{m,l}\mathbb{E}(Z_m Z_l)\cos\phi_m\cos\phi_l \tag{K.173}$$

$$= \frac{2}{M}\sum_{m,l}\frac{1}{2}\delta_{ml}\cos\phi_m\cos\phi_l = \frac{1}{M}\sum_m \cos^2\phi_m = \frac{1}{2}. \tag{K.174}$$

$\mathbb{V}(Y_2)$ is similar. For the covariance,

$$\mathrm{COV}(Y_1, Y_2) = \mathbb{E}\left\{[Y_1 - \mathbb{E}(Y_1)][Y_2 - \mathbb{E}(Y_2)]\right\} = \frac{2}{M}\,\mathbb{E}\left(\sum_m Z_m \cos\phi_m \sum_l Z_l \sin\phi_l\right) \tag{K.175}$$

$$= \frac{2}{M}\sum_{m,l}\mathbb{E}(Z_m Z_l)\cos\phi_m \sin\phi_l = \frac{2}{M}\sum_{m,l}\frac{1}{2}\delta_{ml}\cos\phi_m\sin\phi_l \tag{K.176}$$

$$= \frac{2}{M}\frac{1}{2}\sum_m \cos\phi_m \sin\phi_m = 0. \tag{K.177}$$

Two Gaussian random variables have zero covariance if and only if they are independent. Hence, we can write their probability density as a product of Gaussian probability densities:

$$f(y_1, y_2) = \frac{1}{\sqrt{\pi}}\exp\left[-(y_1 - \mathrm{Re}\,\alpha)^2\right]\frac{1}{\sqrt{\pi}}\exp\left[-(y_2 - \mathrm{Im}\,\alpha)^2\right]. \tag{K.178}$$

(4) We can use the **factorization theorem** (https://en.wikipedia.org/wiki/Sufficient_statistic). Write the probability density of the M outcomes as

$$f \propto \exp\left\{-\sum_m \left[x_m - \sqrt{\frac{2}{M}}\,\mathrm{Re}(\alpha e^{-i\phi_m})\right]^2\right\} \tag{K.179}$$

$$= \exp\left\{-\sum_m \left[x_m^2 - 2x_m\sqrt{\frac{2}{M}}\,\mathrm{Re}(\alpha e^{-i\phi_m}) + \frac{2}{M}[\mathrm{Re}(\alpha e^{-i\phi_m})]^2\right]\right\} \tag{K.180}$$

$$= \exp\left(-\sum_m x_m^2\right)\exp\left\{\sum_m \left[2x_m\sqrt{\frac{2}{M}}\,\mathrm{Re}(\alpha e^{-i\phi_m}) - \frac{2}{M}[\mathrm{Re}(\alpha e^{-i\phi_m})]^2\right]\right\}. \tag{K.181}$$

Notice that we can write

$$\sqrt{\frac{2}{M}}\sum_m x_m\,\mathrm{Re}(\alpha e^{-i\phi_m}) = \sqrt{\frac{2}{M}}\sum_m x_m(\mathrm{Re}\,\alpha\cos\phi_m + \mathrm{Im}\,\alpha\sin\phi_m) \tag{K.182}$$

$$= y_1\,\mathrm{Re}\,\alpha + y_2\,\mathrm{Im}\,\alpha, \tag{K.183}$$

so f can be expressed as

$$f \propto \exp\left(-\sum_m x_m^2\right)\exp\left\{2(y_1\,\mathrm{Re}\,\alpha + y_2\,\mathrm{Im}\,\alpha) - \frac{2}{M}[\mathrm{Re}(\alpha e^{-i\phi_m})]^2\right\}. \tag{K.184}$$

When the probability density is in this form, the factorization theorem says that y_1 and y_2 are sufficient statistics.

Exercise 9.6.

(1) Define a c-number

$$C \equiv \frac{|\alpha|}{\sqrt{2}}(\phi_1 - \phi_2) \tag{K.185}$$

so that we can write

$$\hat{O} = C + \hat{O}_2. \tag{K.186}$$

$\hat{O}_2$ is a quadrature operator for the dark-port input. By Exercise D.6, their orthonormal eigenstates are related by

$$|O = \lambda\rangle = |O_2 = \lambda - C\rangle\,. \tag{K.187}$$

The probability density of $\hat{O}$ is then

$$f_O(\lambda) = \langle O = \lambda|\,\hat{\rho}\,|O = \lambda\rangle = \langle O_2 = \lambda - C|\,\hat{\rho}\,|O_2 = \lambda - C\rangle\,. \tag{K.188}$$

The dark-port input is the vacuum state. We know that the probability density for any quadrature (Exercise 4.26) is

$$\langle O_2 = x|\,\hat{\rho}\,|O_2 = x\rangle = \frac{1}{\sqrt{\pi}}\exp\left(-x^2\right), \tag{K.189}$$

i.e., it is a Gaussian probability density with zero mean and variance equal to $1/2$. $f_O(\lambda)$ is hence

$$f_O(\lambda) = \langle O_2 = \lambda - C|\,\hat{\rho}\,|O_2 = \lambda - C\rangle = \frac{1}{\sqrt{\pi}}\exp\left[-(\lambda - C)^2\right]. \tag{K.190}$$

This is a Gaussian probability density with mean equal to $C \equiv \frac{|\alpha|}{\sqrt{2}}(\phi_1 - \phi_2)$ and variance equal to $1/2$.

(2)

$$\mathbb{E}(O) = C \equiv \frac{|\alpha|}{\sqrt{2}}(\phi_1 - \phi_2), \qquad \frac{\sqrt{2}}{|\alpha|}\,\mathbb{E}(O) = \phi_1 - \phi_2, \tag{K.191}$$

so

$$Y = \frac{\sqrt{2}}{|\alpha|}O \tag{K.192}$$

is unbiased estimator of $\phi_1 - \phi_2$.

(3)

$$\mathbb{E}(Y) = \phi_1 - \phi_2, \qquad \mathbb{V}(Y) = \frac{2}{|\alpha|^2}\,\mathbb{V}(O) = \frac{2}{|\alpha|^2}\frac{1}{2} = \frac{1}{|\alpha|^2}. \tag{K.193}$$

Hence

$$\text{SNR} = \frac{[\mathbb{E}(Y)]^2}{\mathbb{V}(Y)} = |\alpha|^2(\phi_1 - \phi_2)^2. \tag{K.194}$$

(4) With a coherent-state input, the mean of $\hat{O}_2$ becomes

$$\langle O_2\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\theta + i\bar{\phi}}\beta + \text{c.c.}\right), \tag{K.195}$$

and the variance is still $1/2$. The probability density is still Gaussian:

$$\langle O_2 = \lambda|\,\hat{\rho}\,|O_2 = \lambda\rangle = \frac{1}{\sqrt{\pi}}\exp\left[-(\lambda - \langle O_2\rangle)^2\right]. \tag{K.196}$$

The probability density of O becomes

$$f_O(\lambda') = \frac{1}{\sqrt{\pi}}\exp\left[-(\lambda' - C - \langle O_2\rangle)^2\right], \tag{K.197}$$

so O is still a Gaussian random variable, the variance is still $1/2$, but the mean is now $C + \langle O_2 \rangle$.

$$\mathbb{E}(O) = \frac{|\alpha|}{\sqrt{2}}(\phi_1 - \phi_2) + \langle O_2 \rangle\,, \qquad \frac{\sqrt{2}}{|\alpha|}[\mathbb{E}(O) - \langle O_2 \rangle] = \phi_1 - \phi_2. \tag{K.198}$$

So

$$Y = \frac{\sqrt{2}}{|\alpha|}(O - \langle O_2 \rangle) \tag{K.199}$$

is an unbiased estimator.

$$\mathbb{E}(Y) = \phi_1 - \phi_2, \qquad \mathbb{V}(Y) = \frac{2}{|\alpha|^2}\,\mathbb{V}(O) = \frac{1}{|\alpha|^2}, \qquad \text{SNR} = |\alpha|^2(\phi_1 - \phi_2)^2. \tag{K.200}$$

The SNR is exactly the same.

Exercise 9.8. The probability density of a quadrature is

$$\langle O = \lambda |\, \hat{\rho} \,| O = \lambda \rangle = \int \Phi(\alpha) |\langle O = \lambda | \alpha \rangle|^2 d^2\alpha. \tag{K.201}$$

We know $|\langle O = \lambda | \alpha \rangle|^2$ is a Gaussian distribution with some mean and variance equal to $1/2$. Since $\Phi(\alpha)$ is a probability density, we can think of α as a random variable and use the **law of total variance** (see Eq. (C.48)):

$$\mathbb{V}(O) = \mathbb{E}\left[\mathbb{V}(O|\alpha)\right] + \mathbb{V}\left[\mathbb{E}(O|\alpha)\right]. \tag{K.202}$$

$\mathbb{V}(O|\alpha)$ is the variance of O given α, which can be computed from $|\langle O = \lambda | \alpha \rangle|^2$. The result is

$$\mathbb{V}(O|\alpha) = \frac{1}{2}. \tag{K.203}$$

We also know that the variance $\mathbb{V}\left[\mathbb{E}(O|\alpha)\right]$ must always be nonnegative, as long as Φ is a probability density so that α is a classical random variable. Hence

$$\mathbb{V}(O) = \mathbb{E}\left(\frac{1}{2}\right) + \mathbb{V}\left[\mathbb{E}(O|\alpha)\right] = \frac{1}{2} + \mathbb{V}\left[\mathbb{E}(O|\alpha)\right] \geq \frac{1}{2}. \tag{K.204}$$

Exercise 11.1. Note that the main-text definition is equivalent to

$$W(x,y) \equiv \operatorname{tr}\left[\hat{\rho}\hat{W}(x,y)\right], \qquad \hat{W}(x,y) = \frac{1}{(2\pi)^2}\iint e^{i\xi(\hat{q}-x)+i\eta(\hat{p}-y)} d\xi d\eta. \tag{K.205}$$

The alternative definition is

$$W(x,y) = \operatorname{tr}\left[\hat{\rho}\hat{W}'(x,y)\right], \qquad \hat{W}'(x,y) \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\lambda y} \left|q = x + \frac{\lambda}{2}\right\rangle \left\langle q = x - \frac{\lambda}{2}\right| d\lambda. \tag{K.206}$$

We need to show that $\hat{W}(x,y) = \hat{W}'(x,y)$. Use BCH formula to write

$$\begin{aligned}
& e^{i\xi(\hat{q}-x)+i\eta(\hat{p}-y)} \\
&= e^{i\eta(\hat{p}-y)/2} e^{i\xi(\hat{q}-x)} e^{i\eta(\hat{p}-y)/2} && \text{(BCH)} && \text{(K.207)} \\
&= \int_{-\infty}^{\infty} e^{i\eta(\hat{p}-y)/2} e^{i\xi(\lambda-x)} \,|q=\lambda\rangle\langle q=\lambda|\, e^{i\eta(\hat{p}-y)/2} d\lambda && \text{(diagonal form of } \hat{q}) && \text{(K.208)} \\
&= \int_{-\infty}^{\infty} e^{i\eta(-y)/2} e^{i\xi(\lambda-x)} \left|q = \lambda - \frac{\eta}{2}\right\rangle \left\langle q = \lambda + \frac{\eta}{2}\right| e^{i\eta(-y)/2} d\lambda \quad \left(e^{i\eta\hat{p}/2}\,|q=\lambda\rangle = \left|q = \lambda - \frac{\eta}{2}\right\rangle\right) && \text{(K.209)} \\
&= \int_{-\infty}^{\infty} e^{-i\eta y} e^{i\xi(\lambda-x)} \left|q = \lambda - \frac{\eta}{2}\right\rangle \left\langle q = \lambda + \frac{\eta}{2}\right| d\lambda. && && \text{(K.210)}
\end{aligned}$$

Now $\hat{W}(x,y)$ is equal to

$$\hat{W}(x,y) = \frac{1}{(2\pi)^2}\iint e^{i\xi(\hat{q}-x)+i\eta(\hat{p}-y)}d\xi d\eta \tag{K.211}$$

$$= \frac{1}{2\pi}\iint e^{-i\eta y}\delta(\lambda-x)\left|q=\lambda-\frac{\eta}{2}\right\rangle\left\langle q=\lambda+\frac{\eta}{2}\right| d\lambda d\eta \qquad \left(\int_{-\infty}^{\infty} e^{i\xi(\lambda-x)}d\xi = 2\pi\delta(\lambda-x)\right) \tag{K.212}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\eta y}\left|q=x-\frac{\eta}{2}\right\rangle\left\langle q=x+\frac{\eta}{2}\right| d\eta \tag{K.213}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\lambda y}\left|q=x+\frac{\lambda}{2}\right\rangle\left\langle q=x-\frac{\lambda}{2}\right| d\lambda = \hat{W}'(x,y). \qquad \text{(substitute } \lambda=-\eta\text{)} \tag{K.214}$$

Exercise 11.4. Rewrite $\chi(\xi,\eta)$ as

$$\chi(\xi,\eta) = \operatorname{tr}\{\hat{\rho}\exp\{i\xi[\hat{q}(\theta)\cos\theta - \hat{p}(\theta)\sin\theta] + i\eta[\hat{q}(\theta)\sin\theta + \hat{p}(\theta)\cos\theta]\}\} \tag{K.215}$$

$$= \operatorname{tr}\left\{\hat{\rho}\exp\left[i\xi'\hat{q}(\theta) + i\eta'\hat{p}(\theta)\right]\right\} \equiv \chi'(\xi',\eta'), \tag{K.216}$$

where

$$\xi' = \xi\cos\theta + \eta\sin\theta, \qquad \eta' = -\xi\sin\theta + \eta\cos\theta. \tag{K.217}$$

Now do a change of variables in the following integral:

$$W(x,y) \equiv \frac{1}{(2\pi)^2}\iint \chi(\xi,\eta)\exp(-i\xi x - i\eta y)d\xi d\eta \tag{K.218}$$

$$= \frac{1}{(2\pi)^2}\iint \chi'(\xi',\eta')\exp\left[-i(\xi'\cos\theta - \eta'\sin\theta)x - i(\xi'\sin\theta + \eta'\cos\theta)y\right]d\xi' d\eta' \tag{K.219}$$

$$= \frac{1}{(2\pi)^2}\iint \chi'(\xi',\eta')\exp\left(-i\xi' u - i\eta' v\right)d\xi' d\eta', \tag{K.220}$$

where

$$u = x\cos\theta + y\sin\theta, \qquad v = -x\sin\theta + y\cos\theta. \tag{K.221}$$

It follows that

$$W(x,y) = W'(u,v) = \frac{1}{(2\pi)^2}\iint \chi'(\xi',\eta')\exp\left(-i\xi' u - i\eta' v\right)d\xi' d\eta'. \tag{K.222}$$

Now consider

$$\int_{-\infty}^{\infty} W'(u,v)dv$$

$$= \frac{1}{(2\pi)^2}\iint \chi'(\xi',\eta')\exp\bigl(-i\xi' u\bigr)2\pi\delta(\eta')d\xi' d\eta' \qquad \left(\int_{-\infty}^{\infty} e^{-i\eta' v}dv = 2\pi\delta(\eta')\right) \tag{K.223}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \chi'(\xi',0)\exp\bigl(-i\xi' u\bigr)d\xi' \tag{K.224}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \operatorname{tr}\left\{\hat{\rho}\exp\bigl[i\xi'\hat{q}(\theta)\bigr]\right\}\exp\bigl(-i\xi' u\bigr)d\xi' \qquad \text{(from Eq. (K.216))} \tag{K.225}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle q(\theta)=\lambda|\,\hat{\rho}\,|q(\theta)=\lambda\rangle\exp\bigl(i\xi'\lambda\bigr)d\lambda\exp\bigl(-i\xi' u\bigr)d\xi' \qquad \text{(used diagonal form of } \hat{q}(\theta)) \tag{K.226}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle q(\theta)=\lambda|\,\hat{\rho}\,|q(\theta)=\lambda\rangle\, 2\pi\delta(\lambda-u)d\lambda \qquad \left(\int_{-\infty}^{\infty} e^{i\xi'(\lambda-u)}d\xi' = 2\pi\delta(\lambda-u)\right) \tag{K.227}$$

$$= \langle q(\theta)=u|\,\hat{\rho}\,|q(\theta)=u\rangle\,. \tag{K.228}$$

The derivation of $\int_{-\infty}^{\infty} W'(u,v)du = \langle p(\theta)=v|\,\hat{\rho}\,|p(\theta)=v\rangle$ is similar.

Exercise B.39. For any $\hat{A}$ on $\mathcal{H}_A$,

$$\operatorname{tr}\left\{\hat{A}\operatorname{tr}_B\left[\left(\hat{I}\otimes\hat{B}\right)\hat{O}\right]\right\} = \operatorname{tr}\left[\left(\hat{A}\otimes\hat{I}\right)\left(\hat{I}\otimes\hat{B}\right)\hat{O}\right] \qquad \text{(definition of partial trace)} \tag{K.229}$$

$$= \operatorname{tr}\left[\left(\hat{I}\otimes\hat{B}\right)\left(\hat{A}\otimes\hat{I}\right)\hat{O}\right] \qquad ([\hat{A}\otimes\hat{I},\hat{I}\otimes\hat{B}]=0) \tag{K.230}$$

$$= \operatorname{tr}\left[\left(\hat{A}\otimes\hat{I}\right)\hat{O}\left(\hat{I}\otimes\hat{B}\right)\right] \qquad \text{(cyclic property of trace)} \tag{K.231}$$

$$= \operatorname{tr}\left\{\hat{A}\operatorname{tr}_B\left[\hat{O}\left(\hat{I}\otimes\hat{B}\right)\right]\right\}. \qquad \text{(definition of partial trace)} \tag{K.232}$$

It can be proved that $\operatorname{tr}\left(\hat{A}\hat{B}\right) = \operatorname{tr}\left(\hat{A}\hat{C}\right)$ for all $\hat{A}$ if and only if $\hat{B}=\hat{C}$. The desired result follows.

Exercise B.40. For any $\hat{A}$ on $\mathcal{H}_A$,

$$\operatorname{tr}\left[\hat{A}\hat{A}_1\left(\operatorname{tr}_B\hat{O}\right)\hat{A}_2\right] = \operatorname{tr}\left[\hat{A}_2\hat{A}\hat{A}_1\left(\operatorname{tr}_B\hat{O}\right)\right] \qquad \text{(cyclic property)} \tag{K.233}$$

$$= \operatorname{tr}\left\{\left[(\hat{A}_2\hat{A}\hat{A}_1)\otimes\hat{I}\right]\hat{O}\right\} \qquad \text{(definition of partial trace)} \tag{K.234}$$

$$= \operatorname{tr}\left[\left(\hat{A}\otimes\hat{I}\right)\left(\hat{A}_1\otimes\hat{I}\right)\hat{O}\left(\hat{A}_2\otimes\hat{I}\right)\right] \qquad \text{(cyclic property)} \tag{K.235}$$

$$= \operatorname{tr}\left\{\hat{A}\operatorname{tr}_B\left[\left(\hat{A}_1\otimes\hat{I}\right)\hat{O}\left(\hat{A}_2\otimes\hat{I}\right)\right]\right\}. \qquad \text{(definition of partial trace)} \tag{K.236}$$

Exercise D.6.

(1) Apply $\hat{B}$ to $|A=\lambda\rangle$:

$$\hat{B}\,|A=\lambda\rangle = (a\hat{A}+b)\,|A=\lambda\rangle = (a\lambda+b)\,|A=\lambda\rangle\,. \tag{K.237}$$

It follows that $|A=\lambda\rangle$ is an eigenstate of $\hat{B}$ with eigenvalue $u=(a\lambda+b)$. Then we know that

$$|B=u\rangle \propto |A=(u-b)/a\rangle\,. \tag{K.238}$$

Let $|B=u\rangle = z\,|A=(u-b)/a\rangle$, where z is a complex c-number. The orthonormality requires

$$\big\langle B=u\big|B=u'\big\rangle = |z|^2\,\big\langle A=(u-b)/a\big|A=(u'-b)/a\big\rangle \tag{K.239}$$

$$= |z|^2\delta(u/a-u'/a) = |z|^2|a|\delta(u-u') = \delta(u-u'). \tag{K.240}$$

It follows that we must have $|z|=1/\sqrt{|a|}$, and

$$\boxed{|B=u\rangle = \frac{e^{i\angle z}}{\sqrt{|a|}}\,|A=(u-b)/a\rangle\,,} \tag{K.241}$$

where $\angle z$ can be set as any real number. Now derive the completeness condition:

$$\int_{-\infty}^{\infty} |B=u\rangle\,\langle B=u|\,du$$

$$= |z|^2\int_{-\infty}^{\infty} |A=(u-b)/a\rangle\,\langle A=(u-b)/a|\,du \tag{K.242}$$

$$= \frac{1}{|a|}\begin{cases}\int_{-\infty}^{\infty}|A=\lambda\rangle\,\langle A=\lambda|\,ad\lambda, & a>0\\ \int_{\infty}^{-\infty}|A=\lambda\rangle\,\langle A=\lambda|\,ad\lambda, & a<0\end{cases} \qquad (\lambda=(u-b)/a) \tag{K.243}$$

$$= \int_{-\infty}^{\infty}|A=\lambda\rangle\,\langle A=\lambda|\,d\lambda = \hat{I}. \qquad (\{|A=\lambda\rangle\}\text{ is complete}) \tag{K.244}$$

(2)

$$f_B(u) = |\langle B=u|\psi\rangle|^2 = |z\,\langle A=(u-b)/a|\psi\rangle|^2 = \boxed{\frac{1}{|a|}f_A((u-b)/a).} \tag{K.245}$$

This is the same as the probability density after a change of the random variable from A to $B=aA+b$.

APPENDIX L

List of Common Symbols and Notations

(1) We assume **SI units**, unless otherwise stated.
(2) We use Greek letters a lot; see https://en.wikipedia.org/wiki/Greek_alphabet.
(3) Symbols will be recycled a lot. For example,
   (a) the symbol A may denote the vector potential, a matrix, or an operator.
   (b) β may refer to the inverse temperature or a complex amplitude.
   (c) T may refer to the temperature or a time.
   (d) P may be a probability distribution, a polarization field $\boldsymbol{P}(\boldsymbol{r},t)$ in classical EM, or a quadrature operator $\hat{P}$.

Symbol/Notation	Explanation	Examples
$=$	is equal to	
$\equiv$	is defined as	$\hat{U}(t) \equiv \exp\left(-\frac{i}{\hbar}\hat{H}t\right)$
$\leq$	less than or equal to	$0 \leq 0$, $0 \leq 1$
$\geq$	greater than or equal to	$0 \geq 0$, $1 \geq 0$
$<$	strictly less than	
$>$	strictly greater than	

TABLE 1. Basics.

Symbol/Notation	Explanation	Examples
$\mathbb{R}$	All real numbers	0, 1, -1, e, π
$\mathbb{C}$	All complex numbers	$i \equiv \sqrt{-1}$
$\mathbb{N}_0$	All natural numbers including 0	$0, 1, 2, \ldots$
$\mathbb{Z}$	All integers	$\cdots -2, -1, 0, 1, 2, \ldots$
$\{\cdots : \ldots\}$	Unordered set	$\{\sum_{n=1}^{N} \psi_n \left\|e_n\right\rangle : \text{each } \psi_n \in \mathbb{C}\}$
$(\ldots)$	ordered set or row vector	$(\boldsymbol{k}, s)$
$\{\ldots\} \times \{\ldots\}$	Cartesian product of sets	$\mathbb{R} \times \mathbb{R} \equiv \{(x,y) : x \in \mathbb{R} \text{ and } y \in \mathbb{R}\}$
set^n	Cartesian power	$\mathbb{R}^3 \equiv \mathbb{R} \times \mathbb{R} \times \mathbb{R}$
$\in$	belongs to a set	$\left\|\psi\right\rangle \in \mathcal{H}$
$\forall$	"for all" or "for any"	$\langle\psi\|\phi\rangle = (\langle\phi\|\psi\rangle)^* \; \forall \left\|\psi\right\rangle, \left\|\phi\right\rangle \in \mathcal{H}$

TABLE 2. Sets.

Symbol/Notation	Explanation
$\delta_{nm} \equiv \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases}$	Kronecker delta
$\delta^n(\boldsymbol{u})$	n-dimensional Dirac delta
$\lvert z \rvert$	magnitude of a complex number
$\angle z$	phase of a complex number, $z = \lvert z \rvert \exp(i \angle z)$
$\mathrm{Re}\, z \equiv (z + z^*)/2$	real part
$\mathrm{Im}\, z \equiv (z - z^*)/(2i)$	imaginary part
c.c.	complex conjugate
$\mathrm{rect}\, X \equiv \begin{cases} 1, & \lvert X \rvert \leq 1/2 \\ 0, & \lvert X \rvert > 1/2 \end{cases}$	rectangle
$\mathrm{sinc}\, X \equiv \begin{cases} \frac{\sin(\pi X)}{\pi X}, & X \neq 0, \\ 1, & X = 0 \end{cases}$	sinc
$\cosh X \equiv \frac{1}{2}\left(e^X + e^{-X}\right)$	hyperbolic cosine
$\sinh X \equiv \frac{1}{2}\left(e^X - e^{-X}\right)$	hyperbolic sine

TABLE 3. Common functions.

Symbol/Notation	Explanation	Examples
bold symbol	vector in real 3D space	$\boldsymbol{k}$, $\boldsymbol{r}$
tilde $\sim$	unit vector	$\tilde{\boldsymbol{x}}$, $\tilde{\boldsymbol{y}}$, $\tilde{\boldsymbol{z}}$
$\boldsymbol{u} \cdot \boldsymbol{v}$	dot product	$\boldsymbol{k} \cdot \boldsymbol{r}$
$\boldsymbol{u} \times \boldsymbol{v}$	cross product	$\boldsymbol{E} \times \boldsymbol{B}$
$\nabla\cdot$	divergence	$\nabla \cdot \boldsymbol{E}$
$\nabla\times$	curl	$\nabla \times \boldsymbol{E}$
$d^3\boldsymbol{r}$	3D volume element	$d^3\boldsymbol{r} = dxdydz$, $d^3\boldsymbol{k} = dk_x dk_y dk_z$

TABLE 4. Vector calculus.

Symbol/Notation	Explanation	Examples
bold symbol	column vector or row vector	$\boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$, $\boldsymbol{n} = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix}$
$\top$	transpose	$\begin{pmatrix} a & b \end{pmatrix}^\top = \begin{pmatrix} a \\ b \end{pmatrix}$
dagger $\dagger$	conjugate transpose	$\boldsymbol{\alpha}^\dagger = \begin{pmatrix} \alpha_1^* & \alpha_2^* \end{pmatrix}$
star $*$	entry-wise complex conjugate	$\boldsymbol{\alpha}^* = \begin{pmatrix} \alpha_1^* \\ \alpha_2^* \end{pmatrix}$
inverse A^{-1}	matrix inverse	Γ^{-1}
absolute sign $\lvert \ldots \rvert$	vector norm	$\lvert \boldsymbol{\alpha} \rvert^2 = \sum_j \lvert \alpha_j \rvert^2$

TABLE 5. Matrix algebra

Symbol/Notation	Explanation
$\boldsymbol{r} = x\tilde{\boldsymbol{x}} + y\tilde{\boldsymbol{y}} + z\tilde{\boldsymbol{z}}$	3D position vector
$\boldsymbol{k} = k_x\tilde{\boldsymbol{x}} + k_y\tilde{\boldsymbol{y}} + k_z\tilde{\boldsymbol{z}}$	wavevector
$\tilde{\boldsymbol{e}}_{\boldsymbol{k},s}$	polarization vector
$\boldsymbol{E}(\boldsymbol{r}, t)$	electric field
$\boldsymbol{B}(\boldsymbol{r}, t)$	magnetic field
$\boldsymbol{A}(\boldsymbol{r}, t)$	vector potential
$\rho(\boldsymbol{r}, t)$	charge density
$\boldsymbol{J}(\boldsymbol{r}, t)$	current density
$\boldsymbol{P}(\boldsymbol{r}, t)$	polarization field
$\boldsymbol{D}(\boldsymbol{r}, t)$	displacement field
ϵ_0	free-space permittivity
μ_0	free-space permeability
$c \equiv 1/\sqrt{\epsilon_0\mu_0}$	speed of light
$j = (\boldsymbol{k}, s)$	label of a normal mode for free EM fields

TABLE 6. Electromagnetism.

Symbol/Notation	Explanation	Examples
ket $\lvert\ldots\rangle$	Vector in Hilbert space	$\lvert\psi\rangle$
bra $\langle\ldots\rvert$	Adjoint of ket	$\langle\psi\rvert$
bra-ket $\langle\ldots\rvert\ldots\rangle$	Inner product	$\langle\psi\rvert\phi\rangle$
$(\ldots,\ldots)$ or $\langle\ldots,\ldots\rangle$	Inner product (mathematicians' notation)	(ψ,ϕ), $\langle\psi,\phi\rangle$
ket-bra $\lvert\ldots\rangle\langle\ldots\rvert$	Operator in ket-bra form	$\hat{A} = \sum_{n,m} A_{nm}\lvert e_n\rangle\langle e_m\rvert$
hat $\hat{}$	Operator	$\hat{A}$, $\hat{a}$
dagger †	adjoint	$\hat{A}^\dagger$, $\langle\psi\rvert = \lvert\psi\rangle^\dagger$
$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$	Commutator	$[\hat{a}, \hat{a}^\dagger] = 1$
c-number	classical numbers that commute with everything	c, ϵ_0, $\hbar$, ω_j, $\boldsymbol{k}$, A_{nm}
$\mathcal{H}$	Hilbert space	$\{\sum_{n=1}^{N}\psi_n\lvert e_n\rangle$: each $\psi_n \in \mathbb{C}\}$
$\otimes$	Tensor product	$\lvert\psi\rangle\otimes\lvert\phi\rangle$, $\mathcal{H}_A\otimes\mathcal{H}_B$, $\hat{A}\otimes\hat{B}$
$\oplus$	Direct sum	$\boldsymbol{a}\oplus\boldsymbol{b} \equiv \begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\end{pmatrix}$, $A\oplus B \equiv \begin{pmatrix}A & \\ & B\end{pmatrix}$
H.c.	Hermitian conjugate	$\alpha\hat{a}^\dagger - \text{H.c.} = \alpha\hat{a}^\dagger - \alpha^*\hat{a}$
$\hat{I}$	identity operator on $\mathcal{H}$	
$\hat{I}_x$	identity operator on $\mathcal{H}_x$	$\hat{I}_B$ on $\mathcal{H}_B$
$\sim$	Isomorphic relation	$\mathcal{H}_1\otimes\mathcal{H}_2 \sim \mathcal{H}_2\otimes\mathcal{H}_1$
$\hat{A} \geq 0$	$\hat{A}$ is positive-semidefinite	$\hat{\rho}$, $\hat{I}$
$\hat{A} \geq \hat{B}$	$\hat{A} - \hat{B}$ is positive-semidefinite	

TABLE 7. Hilbert space and the bra-ket notation.

Symbol/Notation	Explanation
$\hbar \equiv h/(2\pi)$	Planck constant divided by 2π
$\hat{H}$	Hamiltonian operator
$\hat{U}(t) \equiv \exp\left(-\frac{i}{\hbar}\hat{H}t\right)$	unitary operator
$\hat{\rho}$	density operator
$\langle A \rangle \equiv \mathrm{tr}(\hat{A}\hat{\rho})$	expected value
$\left\langle \Delta A^2 \right\rangle \equiv \mathrm{tr}(\hat{A}^2\hat{\rho}) - [\mathrm{tr}(\hat{A}\hat{\rho})]^2$	variance
Z	partition function
$\beta \equiv 1/k_B T$	inverse temperature

TABLE 8. Quantum.

Symbol/Notation	Explanation
$\hat{a}$	annihilation operator
$\hat{n} \equiv \hat{a}^\dagger \hat{a}$	number operator
$\hat{q} \equiv (\hat{a} + \hat{a}^\dagger)/\sqrt{2}$	q-quadrature operator
$\hat{p} \equiv (\hat{a} - \hat{a}^\dagger)/(\sqrt{2}i)$	p-quadrature operator
$\lvert n \rangle$	eigenstate of $\hat{n}$ with eigenvalue n
$\lvert q = x \rangle$	eigenstate of $\hat{q}$ with eigenvalue x
$\lvert p = y \rangle$	eigenstate of $\hat{p}$ with eigenvalue y
$\lvert \alpha \rangle$ (with greek letter $\alpha, \beta, \ldots$ as argument)	coherent state, $\alpha \in \mathbb{C}$
$\hat{D}(\alpha)$	displacement operator
$d^2\alpha$	$(d\,\mathrm{Re}\,\alpha)(d\,\mathrm{Im}\,\alpha)$
$\Phi(\alpha)$	Sudarshan representation, also called P function

TABLE 9. Single-mode algebra.

Symbol/Notation	Explanation
$\lvert \boldsymbol{\alpha} \rangle$	multimode coherent state, $\boldsymbol{\alpha} \in \mathbb{C}^J$
$\hat{D}(\boldsymbol{\alpha})$	multimode displacement operator
$d^{2J}\boldsymbol{\alpha}$	$\prod_{j=1}^{J}(d\,\mathrm{Re}\,\alpha_j)(d\,\mathrm{Im}\,\alpha_j)$
$\Phi(\boldsymbol{\alpha})$	Sudarshan representation, also called P function
$\hat{a}_j, \hat{n}_j, \hat{q}_j, \hat{p}_j$	Operators for mode j
$\lvert q = \boldsymbol{x} \rangle$	eigenstate of $\{\hat{q}_j\}$, $\hat{q}_j \lvert q = \boldsymbol{x} \rangle = x_j \lvert q = \boldsymbol{x} \rangle$
$\lvert p = \boldsymbol{y} \rangle$	eigenstate of $\{\hat{p}_j\}$, $\hat{p}_j \lvert p = \boldsymbol{y} \rangle = y_j \lvert p = \boldsymbol{y} \rangle$
$\lvert \boldsymbol{n} \rangle \equiv \lvert n_1, \ldots, n_J \rangle$	multimode number state

TABLE 10. Multimode algebra.

Symbol/Notation	Explanation
Ω	sample space
F or E	event space
(Ω, F, P)	probability space
$P_X \otimes P_Y$	product measure
i.i.d.	independent and identically distributed
$P^{\otimes n}$	tensor product of n identical meaures P for i.i.d. variables
$P_{X_1,\ldots,X_n}(x_1, \ldots, x_n)$	joint probability distribution
$f_{X_1,\ldots,X_n}(x_1, \ldots, x_n)$	joint probability density
$P[A\|B]$	conditional probability
$\mathbb{E}(X)$	expected value of a random variable X
$\mathbb{V}(X) \equiv \mathbb{E}\left\{[X - \mathbb{E}(X)]^2\right\} = \mathbb{E}(X^2) - [\mathbb{E}(X)]^2$	variance
$\mathrm{COV}(X, Y) \equiv \mathbb{E}\{[X - \mathbb{E}(X)][Y - \mathbb{E}(Y)]\} = \mathbb{E}(XY) - [\mathbb{E}(X)][\mathbb{E}(Y)]$	covariance
$C(\tau)$	covariance function
$S(\omega)$	power spectral density
$\frac{dP}{dQ}(x)$	Radon-Nikodym derivative

TABLE 11. Probability.

Symbol/Notation	Explanation
$\hat{\rho}$	density operator
$\hat{\Pi}$	projection-valued measure (PVM)
$\hat{M}$	positive operator-valued measure (POVM)
$\mathcal{F}$	completely positive (CP) map
$\mathcal{F}(S)\hat{\rho}$	hybrid state
$\hat{\rho}_S \equiv \mathcal{F}(S)\hat{\rho}/\operatorname{tr}(\text{numerator})$	posterior state

TABLE 12. Open quantum systems.

Symbol/Notation	Explanation
$S \equiv \begin{pmatrix} \tau & r \\ r' & \tau' \end{pmatrix}$	scattering matrix
$\chi^{(1)}$	linear optical susceptibility
$\chi^{(2)}$	second-order optical susceptibility

TABLE 13. Optics.

Symbol	Concept	Other names
$\theta \in \Theta$	parameter	hypothesis
Θ	parameter space	
$\{P_\theta : \theta \in \Theta\}$	statistical model	
$f_\theta(x) \equiv \frac{dP_\theta}{d\sigma}(x)$	probability density	Radon-Nikodym derivative
$\mathbb{E}_\theta$	Expectation with respect to P_θ	
$\check{\theta}$	decision rule	estimator
$l(\theta, \check{\theta})$	loss function	error function, cost function
$R(\theta, \check{\theta}) \equiv \mathbb{E}_\theta \left[l(\theta, \check{\theta}) \right]$	error	expected loss, risk function
π	prior probability measure	
$R_\pi(\check{\theta}) \equiv \int R(\theta, \check{\theta}) d\pi(\theta)$	average error	average risk
$\check{\theta}_{\text{Bayes}} \equiv \arg\min_{\check{\theta}} R_\pi(\check{\theta})$	Bayes rule	Bayes estimator
$R_{\text{Bayes}}(\pi) \equiv \min_{\check{\theta}} R_\pi(\check{\theta}) = R_\pi(\check{\theta}_{\text{Bayes}})$	Bayes error	Bayes risk
$\max_{\theta \in \Theta} R(\theta, \check{\theta})$	worst-case error	worst-case risk
$\check{\theta}_{\text{minimax}} \equiv \arg\min_{\check{\theta}} \max_{\theta \in \Theta} R(\theta, \check{\theta})$	minimax rule	minimax estimator
$\min_{\check{\theta}} \max_{\theta \in \Theta} R(\theta, \check{\theta}) = \max_{\theta \in \Theta} R(\theta, \check{\theta}_{\text{minimax}})$	minimax error	minimax risk

TABLE 14. Statistics.

Symbol	Concept	Other names
$R_{\text{NP}}(\alpha)$	Neyman-Pearson error given tolerance level α	
$\Lambda(x) \equiv \frac{dP_1}{dP_0}(x)$	likelihood ratio	Radon-Nikodym derivative
$\lambda(x) \equiv \ln \Lambda(x)$	log-likelihood ratio	
$\Lambda \gtrless T$, $\lambda \gtrless t$	likelihood-ratio test with threshold T or t	
K	Kolmogorov distance	
$\mu(s) \equiv \ln \mathbb{E}_0(\Lambda^s)$	Chebyshev exponent	
$C \equiv \max_{0<s<1}[-\mu(s)]$	Chernoff distance	Chernoff exponent
$D(P_1 \| P_0)$	relative entropy	Kullback-Leibler divergence
$B \equiv -\mu(1/2)$	Bhattacharyya distance	(closely related to Hellinger distance)

TABLE 15. Binary hypothesis testing.

Symbol	Concept	Other names
$\beta(\theta)$	key parameter	parameter of interest
$G(v)$	Gill-Levit bound	Bayesian Cramér-Rao bounds, Van Trees inequalities
$\nabla \equiv \left(\frac{\partial}{\partial\theta_1} \quad \cdots \quad \frac{\partial}{\partial\theta_p}\right)^\top$	gradient with respect to θ	
$F(\theta)$	Fisher information	information
$\mathsf{C}(\theta)$	Cramér-Rao bound (CRB)	information inequality
$\check{\theta}_{\mathrm{ML}}(x)$, $\check{\beta}_{\mathrm{ML}}(x)$	maximum-likelihood (ML) estimator	
$\delta(\theta) \equiv \mathbb{E}_\theta(\check{\beta}) - \beta(\theta)$	bias	
$f_\phi(x)$ given x	likelihood function	
$L_\phi(x) \equiv \ln f_\phi(x)$	log-likelihood function	

TABLE 16. Parameter estimation.

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